

stn

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\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 AUG 15 CAOLD to be discontinued on December 31, 2008  
NEWS 3 OCT 07 EPFULL enhanced with full implementation of EPC2000  
NEWS 4 OCT 07 Multiple databases enhanced for more flexible patent  
number searching  
NEWS 5 OCT 22 Current-awareness alert (SDI) setup and editing  
enhanced  
NEWS 6 OCT 22 WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT  
Applications  
NEWS 7 OCT 24 CHEMLIST enhanced with intermediate list of  
pre-registered REACH substances  
NEWS 8 NOV 21 CAS patent coverage to include exemplified prophetic  
substances identified in English-, French-, German-,  
and Japanese-language basic patents from 2004-present  
NEWS 9 NOV 26 MARPAT enhanced with FSORT command  
NEWS 10 NOV 26 MEDLINE year-end processing temporarily halts  
availability of new fully-indexed citations  
NEWS 11 NOV 26 CHEMSAFE now available on STN Easy  
NEWS 12 NOV 26 Two new SET commands increase convenience of STN  
searching  
NEWS 13 DEC 01 ChemPort single article sales feature unavailable  
  
NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.  
  
NEWS HOURS STN Operating Hours Plus Help Desk Availability  
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\* \* \* \* \* STN Columbus \* \* \* \* \*

Updated Search

stn

FILE 'HOME' ENTERED AT 06:01:08 ON 08 DEC 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 06:01:29 ON 08 DEC 2008

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 5 DEC 2008 HIGHEST RN 1080697-25-1

DICTIONARY FILE UPDATES: 5 DEC 2008 HIGHEST RN 1080697-25-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Documents and Settings\brobinson1\My Documents\342a.str

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 06:03:55 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 356 TO ITERATE

100.0% PROCESSED 356 ITERATIONS 15 ANSWERS

SEARCH TIME: 00.00.05

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5988 TO 8252

PROJECTED ANSWERS: 68 TO 532

L2 15 SEA SSS SAM L1

=> s l1 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 06:04:05 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 6658 TO ITERATE

Updated Search

stn

100.0% PROCESSED 6658 ITERATIONS  
SEARCH TIME: 00.00.01

277 ANSWERS

L3 277 SEA SSS FUL L1

=> file hcaplus  
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
179.74	179.95

FULL ESTIMATED COST

FILE 'HCAPLUS' ENTERED AT 06:04:08 ON 08 DEC 2008  
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FILE COVERS 1907 - 8 Dec 2008 VOL 149 ISS 24  
FILE LAST UPDATED: 7 Dec 2008 (20081207/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 29 L3

=> s l4 and trotter, b?/au

53 TROTTER, B?/AU

L5

4 L4 AND TROTTER, B?/AU

=> d l5, ibib abs hitstr, 1-4

L5 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2006:1252121 HCAPLUS

DOCUMENT NUMBER: 146:142484

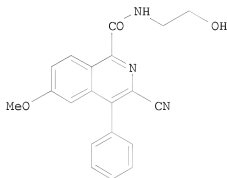
TITLE: Design and Synthesis of Novel Isoquinoline-3-nitriles as Orally Bioavailable Kv1.5 Antagonists for the Treatment of Atrial Fibrillation

AUTHOR(S): Trotter, B. Wesley; Nanda, Kausik K.; Kett, Nathan R.; Regan, Christopher P.; Lynch, Joseph J.; Stump, Gary L.; Kiss, Laszlo; Wang, Jixin; Spencer,

Updated Search

stn

Robert H.; Kane, Stefanie A.; White, Rebecca B.; Zhang, Rena; Anderson, Kenneth D.; Liverton, Nigel J.; McIntyre, Charles J.; Beshore, Douglas C.; Hartman, George D.; Dinsmore, Christopher J. Departments of Medicinal Chemistry, Stroke, and Neurodegeneration Automated Biotechnology Pain Research, and Drug Metabolism, Merck Research Laboratories, West Point, PA, 19486, USA  
CORPORATE SOURCE: Journal of Medicinal Chemistry (2006), 49(24), 6954-6957  
SOURCE: CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 146:142484  
GI

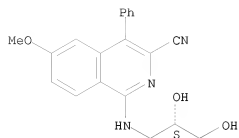


AB Novel 3-cyanoisoquinoline Kv1.5 antagonists have been prepared and evaluated in in vitro and in vivo assays for inhibition of the Kv1.5 potassium channel and its associated cardiac potassium current, I<sub>Kur</sub>. Structural modifications of the isoquinolinone lead afforded compds. (e.g. I) with excellent potency, selectivity, and oral bioavailability.  
IT 849546-23-2P 849546-30-1P 849547-28-0P  
849548-50-1P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation of isoquinoline-3-nitriles as orally bioavailable Kv1.5 antagonists for the treatment of atrial fibrillation)  
RN 849546-23-2 HCAPLUS  
CN 3-Isoquinolinecarbonitrile, 1-[[{(2S)-2,3-dihydroxypropyl}amino]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

Updated Search

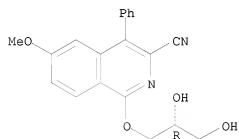
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RN 849546-30-1 HCAPLUS

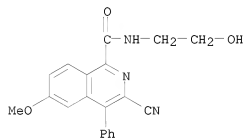
CN 3-Isoquinolinecarbonitrile, 1-[(2R)-2,3-dihydroxypropoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 849547-28-0 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxyethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

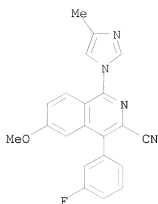


RN 849548-50-1 HCAPLUS

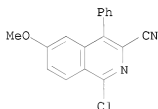
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)

Updated Search

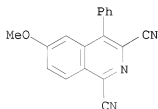
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IT 849546-10-7P 849546-11-8P 849546-26-5P  
 849546-48-1P 849547-30-4P 849549-26-4P  
 849549-27-5P, 4-(3-Fluorophenyl)-6-methoxy-1-oxo-1,2-  
 dihydroisoquinoline-3-carbonitrile  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of isoquinoline-3-nitriles as orally bioavailable Kv1.5  
 antagonists for the treatment of atrial fibrillation)  
 RN 849546-10-7 HCAPLUS  
 CN 3-Isoquinolinecarbonitrile, 1-chloro-6-methoxy-4-phenyl- (CA INDEX NAME)



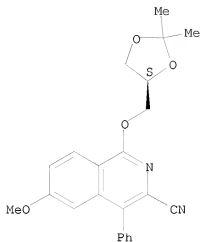
RN 849546-11-8 HCAPLUS  
 CN 1,3-Isoquinolinedicarbonitrile, 6-methoxy-4-phenyl- (CA INDEX NAME)



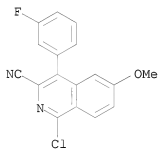
RN 849546-26-5 HCAPLUS  
 CN 3-Isoquinolinecarbonitrile, 1-[[4(S)-2,2-dimethyl-1,3-dioxolan-4-  
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Updated Search

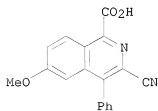
Absolute stereochemistry.



CN	3-Isoquinolinecarbonitrile, 1-chloro-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)	
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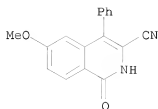
CN 1-Isoquinolinecarboxylic acid, 3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)



CN	3-Isoquinolinecarbonitrile, 1,2-dihydro-6-methoxy-1-oxo-4-phenyl- (CA INDEX NAME)	(CA
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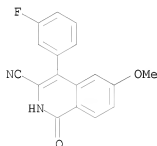
Updated Search

stn



RN 849549-27-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo-  
(CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:300465 HCAPLUS

DOCUMENT NUMBER: 142:373705

TITLE: Preparation of isoquinoline derivatives as potassium  
channel inhibitors

INVENTOR(S): Trotter, B. Wesley; Claiborne, Christopher;  
Ponticello, Gerald S.; McIntyre, Charles J.; Liverton,  
Nigel; Claremon, David A.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030791	A2	20050407	WO 2004-US30431	20040917
WO 2005030791	A3	20050526		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,			

Updated Search



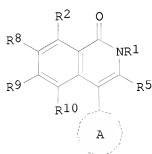
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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,  
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,  
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,  
SN, TD, TG

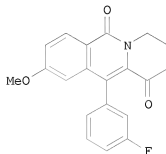
AU 2004276236	A1	20050407	AU 2004-276236	20040917
AU 2004276236	B2	20080124		
CA 2539814	A1	20050407	CA 2004-2539814	20040917
EP 1667982	A2	20060614	EP 2004-788811	20040917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1856476	A	20061101	CN 2004-80027369	20040917
JP 2007516218	T	20070621	JP 2006-528067	20040917
IN 2006DN01030	A	20070817	IN 2006-DN1030	20060227
US 20070027177	A1	20070201	US 2006-571870	20060315
PRIORITY APPLN. INFO.:			US 2003-505101P	P 20030923
			WO 2004-US30431	W 20040917

OTHER SOURCE(S): CASREACT 142:373705; MARPAT 142:373705

GI



I



II

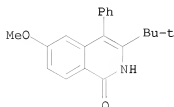
AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl; R1 = H, (cyclo)alkyl, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbonyl, etc.; R5 = H, halo, (cyclo)alkyl, etc.; or R1R5 = (un)substituted cyclic ring; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, reaction of 2-(3-fluorobenzoyl)-4-methoxybenzoyl chloride with piperidin-3-one•HCl gave II. I provide  $\geq 20$  % inhibition at a concentration of 33  $\mu\text{M}$  or less in the high throughput Kv1.5 planar patch clamp assay and  $\geq 25$  % inhibition at a concentration of 25  $\mu\text{M}$  or less in the AAS (Atomic Absorption Spectroscopy) assay. Thus, I and their pharmaceutical compds. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.

IT 849424-93-7P 849424-95-9P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849424-93-7 HCAPLUS

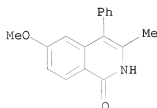
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CN 1 (2H)-Isoquinolinone, 3-(1,1-dimethylethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849424-95-9 HCAPLUS

CN 1 (2H)-Isoquinolinone, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



L5 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:300412 HCAPLUS

DOCUMENT NUMBER: 142:373702

TITLE: Preparation of isoquinoline derivatives as potassium channel inhibitors

INVENTOR(S): Isaacs, Richard; Dinsmore, Christopher J.; Trotter, B. Wesley; Liverton, Nigel; Beshore, Douglas C.; Kett, Nathan R.; McIntyre, Charles J.; Nanda, Kausik K.; Claremon, David A.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 114 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

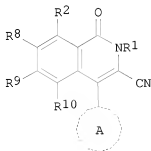
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2005030729	A1	20050407	WO 2004-US30945	20040922
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,			

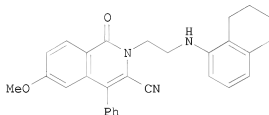
Updated Search

stn

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AU 2004276268	A1	20050407	AU 2004-276268	20040922
CA 2539546	A1	20050407	CA 2004-2539546	20040922
EP 1667981	A1	20060614	EP 2004-784700	20040922
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1856477	A	20061101	CN 2004-80027486	20040922
JP 2007506749	T	20070322	JP 2006-528111	20040922
US 20070054892	A1	20070308	US 2006-572236	20060317
IN 2006DN01544	A	20070810	IN 2006-DN1544	20060322
PRIORITY APPLN. INFO.:			US 2003-505216P	P 20030923
			WO 2004-US30945	W 20040922
OTHER SOURCE(S):			CASREACT 142:373702; MARPAT 142:373702	
GI				



I



II

AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl; R1 = H, (cyclo)alkyl, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbonyl, etc.; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, II was given in a multi-step synthesis starting from the reaction of p-anisoyl chloride with aniline. I provide  $\geq 20$  % inhibition at a concentration of 33  $\mu\text{M}$  or less in the high throughput Kv1.5 planar patch clamp assay and  $\geq 25$  % inhibition at a concentration of 25  $\mu\text{M}$  or less in the AAS (Atomic Absorption Spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.

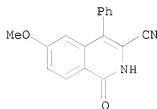
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IT 849549-26-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849549-26-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1,2-dihydro-6-methoxy-1-oxo-4-phenyl- (CA INDEX NAME)



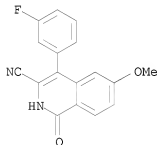
IT 849549-27-5P, 4-(3-Fluorophenyl)-6-methoxy-1-oxo-1,2-dihydroisoquinoline-3-carbonitrile 849549-29-7P,

4-(2-Fluorophenyl)-6-methoxy-1-oxo-1,2-dihydroisoquinoline-3-carbonitrile  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849549-27-5 HCAPLUS

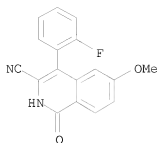
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo- (CA INDEX NAME)



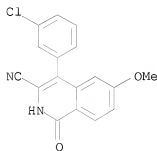
RN 849549-29-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(2-fluorophenyl)-1,2-dihydro-6-methoxy-1-oxo- (CA INDEX NAME)

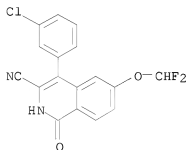
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IT 849635-33-2 849635-44-5  
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL  
(Biological study); USES (Uses)  
(preparation of isoquinoline derivs. as potassium channel inhibitors)  
RN 849635-33-2 HCAPLUS  
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1,2-dihydro-6-methoxy-1-oxo-  
(CA INDEX NAME)



RN 849635-44-5 HCAPLUS  
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-(difluoromethoxy)-1,2-  
dihydro-1-oxo- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN

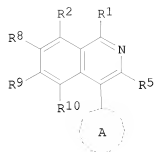
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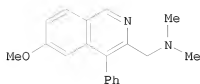
ACCESSION NUMBER: 2005:300191 HCAPLUS  
 DOCUMENT NUMBER: 142:373697  
 TITLE: Preparation of isoquinoline derivatives as potassium channel inhibitors  
 INVENTOR(S): Trotter, B. Wesley; Nanda, Kausik K.; Kett, Nathan R.; Dinsmore, Christopher J.; Ponticello, Gerald S.; Claremon, David A.  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
 SOURCE: PCT Int. Appl., 115 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030130	A2	20050407	WO 2004-US30486	20040917
WO 2005030130	A3	20060119		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2004275720	A1	20050407	AU 2004-275720	20040917
AU 2004275720	B2	20080424		
CA 2539479	A1	20050407	CA 2004-2539479	20040917
EP 1667979	A2	20060614	EP 2004-784370	20040917
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CN 1856475	A	20061101	CN 2004-80027385	20040917
JP 2007506743	T	20070322	JP 2006-528072	20040917
IN 2006DN00877	A	20070810	IN 2006-DN877	20060220
US 20060276450	A1	20061207	US 2006-572342	20060317
PRIORITY APPLN. INFO.:			US 2003-505143P	P 20030923
			WO 2004-US30486	W 20040917
OTHER SOURCE(S):			CASREACT 142:373697; MARPAT 142:373697	
GI				

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I



II

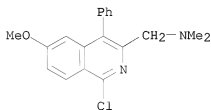
AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl or heterocyclic ring; R1 = H, CN, halo, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbonyl, etc.; R5 = H, halo, (cyclo)alkyl, etc.; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, Ni-catalyzed reduction of 1-chloro-6-methoxy-4-phenylisoquinoline-3-carbonitrile and followed by condensation with formaldehyde, gave II•2HCl. I provided ≥50% inhibition at concentration ≤33 μM in the high-throughput Kv1.5 planar patch clamp assay and ≥25% inhibition at concentration ≤25 μM in the AAS (atomic absorption spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.

IT 849545-74-0P 849545-76-2P 849546-10-7P  
849546-11-8P 849546-13-0P 849546-17-4P  
849546-26-5P 849546-28-7P 849546-48-1P  
849546-58-3P 849547-30-4P 849548-92-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849545-74-0 HCAPLUS

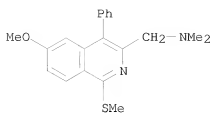
CN 3-Isoquinolinemethanamine, 1-chloro-6-methoxy-N,N-dimethyl-4-phenyl- (CA INDEX NAME)



RN 849545-76-2 HCAPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylthio)-4-phenyl-, hydrochloride (1:2) (CA INDEX NAME)

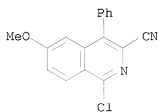
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● 2 HCl

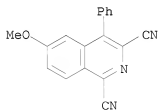
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CN 3-Isoquinolinecarbonitrile, 1-chloro-6-methoxy-4-phenyl- (CA INDEX NAME)



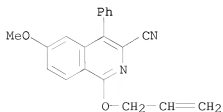
RN 849546-11-8 HCAPLUS

CN 1,3-Isoquinolinedicarbonitrile, 6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-13-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-(2-propen-1-yloxy)- (CA INDEX NAME)



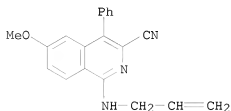
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RN 849546-17-4 HCAPLUS

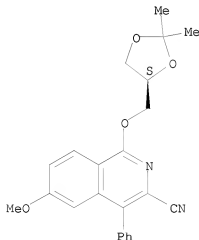
CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-(2-propen-1-ylamino)-  
(CA INDEX NAME)



RN 849546-26-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[ (4S)-2,2-dimethyl-1,3-dioxolan-4-yl]methoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



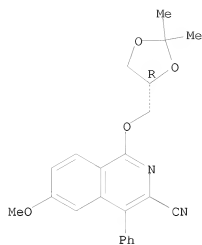
RN 849546-28-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[ (4R)-2,2-dimethyl-1,3-dioxolan-4-yl]methoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

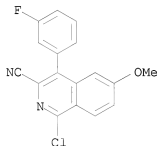
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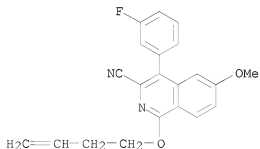
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CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849546-58-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(3-buten-1-yloxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

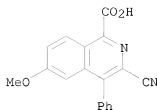


RN 849547-30-4 HCAPLUS

CN 1-Isoquinolinecarboxylic acid, 3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)

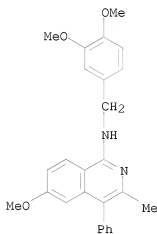
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RN 849548-92-1 HCAPLUS

CN 1-Isoquinolinamine, N-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



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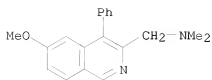
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of isoquinoline derivs. as potassium channel inhibitors)

RN 849545-72-8 HCAPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-4-phenyl-, hydrochloride  
(1:2) (CA INDEX NAME)

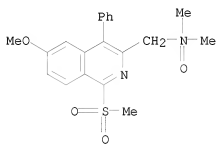
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● 2 HCl

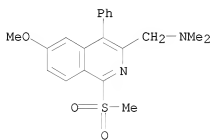
RN 849545-78-4 HCAPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylsulfonyl)-4-phenyl-, N-oxide (CA INDEX NAME)



RN 849545-80-8 HCAPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylsulfonyl)-4-phenyl- (CA INDEX NAME)

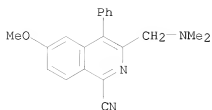


RN 849545-82-0 HCAPLUS

CN 1-Isoquinolinecarbonitrile, 3-[(dimethylamino)methyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

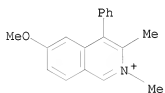
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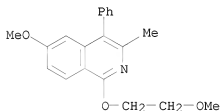
RN 849545-84-2 HCAPLUS

CN Isoquinolinium, 6-methoxy-2,3-dimethyl-4-phenyl-, hydroxide (1:1) (CA INDEX NAME)



RN 849545-86-4 HCAPLUS

CN Isoquinoline, 6-methoxy-1-(2-methoxyethoxy)-3-methyl-4-phenyl- (CA INDEX NAME)

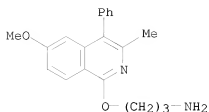


RN 849545-88-6 HCAPLUS

CN 1-Propanamine, 3-[(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)oxy]-, hydrochloride (1:2) (CA INDEX NAME)

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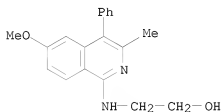
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● 2 HCl

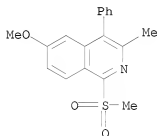
RN 849545-90-0 HCAPLUS

CN Ethanol, 2-[(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)amino]- (CA INDEX NAME)



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CN Isoquinoline, 6-methoxy-3-methyl-1-(methylsulfonyl)-4-phenyl- (CA INDEX NAME)

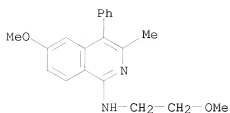


RN 849545-93-3 HCAPLUS

CN 1-Isoquinolinamine, 6-methoxy-N-(2-methoxyethyl)-3-methyl-4-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

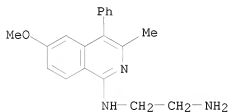
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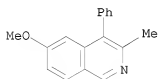
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RN 849545-94-4 HCAPLUS  
CN 1,2-Ethanediamine, N1-(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)-,  
hydrochloride (1:2) (CA INDEX NAME)



●2 HCl

RN 849545-95-5 HCAPLUS  
CN Isoquinoline, 6-methoxy-3-methyl-4-phenyl-, hydrochloride (1:1) (CA INDEX  
NAME)



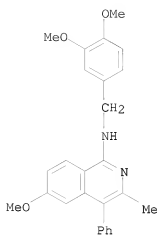
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CN 1-Isoquinolinamine, N-[(3,4-dimethoxyphenyl)methyl]-6-methoxy-3-methyl-4-  
phenyl-, hydrochloride (1:1) (CA INDEX NAME)

Updated Search



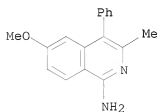
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● HCl

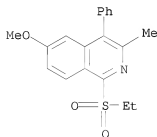
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CN 1-Isoquinolinamine, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



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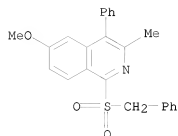


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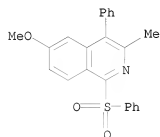
CN Isoquinoline, 6-methoxy-3-methyl-4-phenyl-1-[(phenylmethyl)sulfonyl]- (CA INDEX NAME)

Updated Search

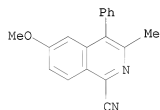
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RN 849546-04-9 HCAPLUS  
CN Isoquinoline, 6-methoxy-3-methyl-4-phenyl-1-(phenylsulfonyl)- (CA INDEX NAME)



RN 849546-06-1 HCAPLUS  
CN 1-Isoquinolinecarbonitrile, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)

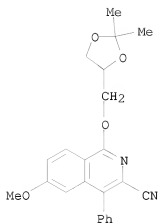


RN 849546-08-3 HCAPLUS  
CN Isoquinoline, 3-(1,1-dimethylethyl)-6-methoxy-1-(2-methoxyethoxy)-4-phenyl- (CA INDEX NAME)

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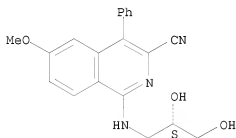
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RN 849546-23-2 HCAPLUS

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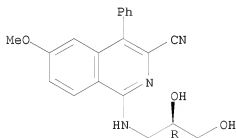
Absolute stereochemistry.



RN 849546-25-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[ (2R)-2,3-dihydroxypropyl]amino]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 849546-30-1 HCAPLUS

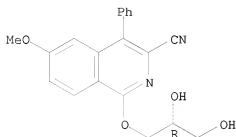
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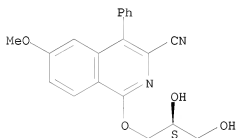
Absolute stereochemistry.



RN 849546-32-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropoxy]-6-methoxy-4-phenyl- (CA INDEX NAME)

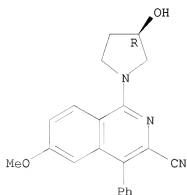
Absolute stereochemistry.



RN 849546-34-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R)-3-hydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



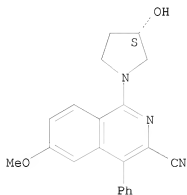
Updated Search

stn

RN 849546-36-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3S)-3-hydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

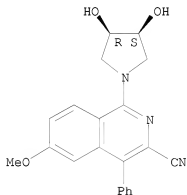
Absolute stereochemistry.



RN 849546-38-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R,4S)-3,4-dihydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl-, rel- (CA INDEX NAME)

Relative stereochemistry.

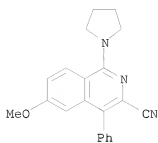


RN 849546-40-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-(1-pyrrolidinyl)- (CA INDEX NAME)

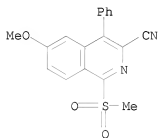
Updated Search

stn



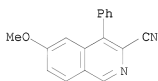
RN 849546-42-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(methylsulfonyl)-4-phenyl- (CA INDEX NAME)



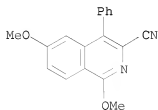
RN 849546-44-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-46-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1,6-dimethoxy-4-phenyl- (CA INDEX NAME)

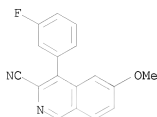


RN 849546-50-5 HCAPLUS

Updated Search

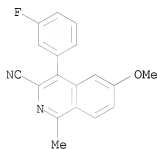
stn

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



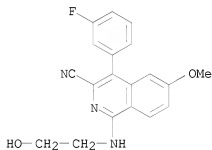
RN 849546-52-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-methyl- (CA INDEX NAME)



RN 849546-54-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[(2-hydroxyethyl)amino]-6-methoxy- (CA INDEX NAME)



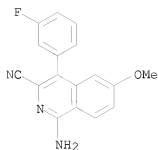
RN 849546-56-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-amino-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Updated Search

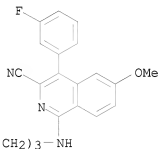


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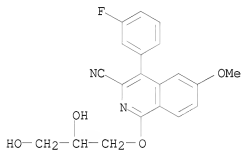
RN 849546-57-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[(3-hydroxypropyl)amino]-6-methoxy- (CA INDEX NAME)



RN 849546-60-7 HCAPLUS

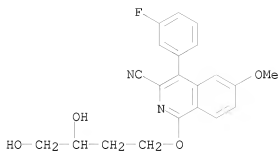
CN 3-Isoquinolinecarbonitrile, 1-(2,3-dihydroxypropoxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849546-63-0 HCAPLUS

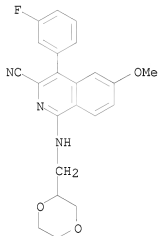
CN 3-Isoquinolinecarbonitrile, 1-(3,4-dihydroxybutoxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

stn



RN 849546-66-3 HCAPLUS

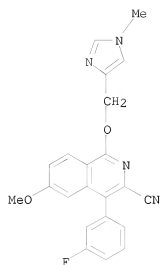
CN 3-Isoquinolinecarbonitrile, 1-[(1,4-dioxan-2-ylmethyl)amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849546-69-6 HCAPLUS

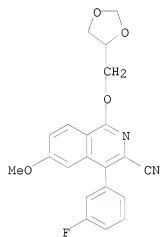
CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-[(1-methyl-1H-imidazol-4-yl)methoxy]- (CA INDEX NAME)

stn



RN 849546-72-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1,3-dioxolan-4-ylmethoxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

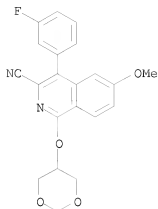


RN 849546-75-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1,3-dioxan-5-yloxy)-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

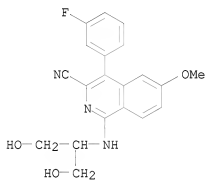
Updated Search

stn



RN 849546-78-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]-6-methoxy- (CA INDEX NAME)

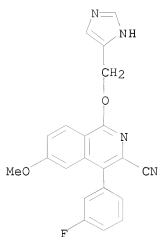


RN 849546-80-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-(1H-imidazol-5-ylmethoxy)-6-methoxy- (CA INDEX NAME)

Updated Search

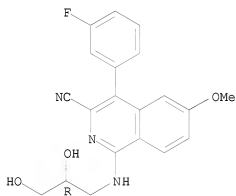
stn



RN 849546-83-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[[(2R)-2,3-dihydroxypropyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



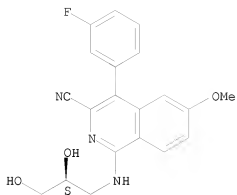
RN 849546-86-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[[(2S)-2,3-dihydroxypropyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

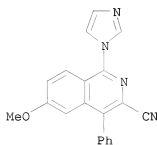
Updated Search

stn



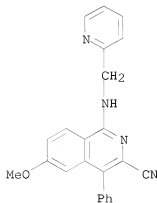
RN 849546-89-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1H-imidazol-1-yl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849546-92-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-[(2-pyridinylmethyl)amino]- (CA INDEX NAME)



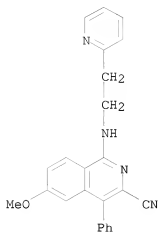
RN 849546-95-8 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-[[2-(2-

Updated Search

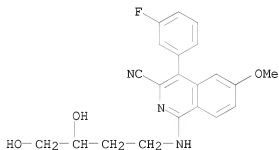
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pyridinyl)ethyl]amino]- (CA INDEX NAME)



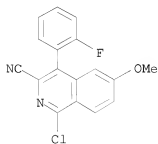
RN 849546-98-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3,4-dihydroxybutyl)amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849547-01-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-chloro-4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)

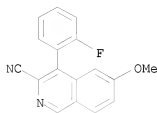


RN 849547-03-1 HCAPLUS

Updated Search

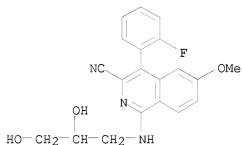
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CN 3-Isoquinolinecarbonitrile, 4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849547-05-3 HCAPLUS

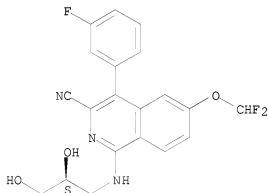
CN 3-Isoquinolinecarbonitrile, 1-[(2,3-dihydroxypropyl)amino]-4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849547-07-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-(difluoromethoxy)-1-[(2S)-2,3-dihydroxypropyl]amino]-4-(3-fluorophenyl)- (CA INDEX NAME)

Absolute stereochemistry.



RN 849547-09-7 HCAPLUS

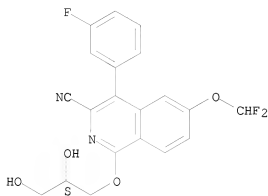
CN 3-Isoquinolinecarbonitrile, 6-(difluoromethoxy)-1-[(2S)-2,3-dihydroxypropoxy]-4-(3-fluorophenyl)- (CA INDEX NAME)

Updated Search



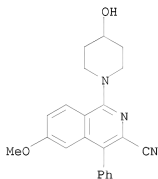
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Absolute stereochemistry.



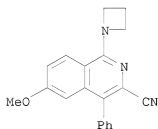
RN 849547-10-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(4-hydroxy-1-piperidiny)-6-methoxy-4-phenyl-  
(CA INDEX NAME)



RN 849547-13-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(1-azetidiny)-6-methoxy-4-phenyl- (CA  
INDEX NAME)



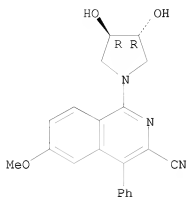
RN 849547-15-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(3R,4R)-3,4-dihydroxy-1-pyrrolidinyl]-6-  
methoxy-4-phenyl- (CA INDEX NAME)

Updated Search

stn

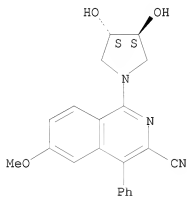
Absolute stereochemistry.



RN 849547-17-7 HCAPLUS

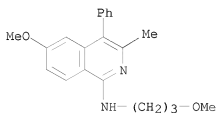
CN 3-Isoquinolinecarbonitrile, 1-[(3S,4S)-3,4-dihydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.



RN 849547-19-9 HCAPLUS

CN 1-Isoquinolinamine, 6-methoxy-N-(3-methoxypropyl)-3-methyl-4-phenyl- (CA INDEX NAME)

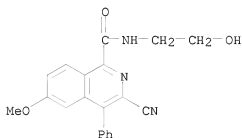


Updated Search

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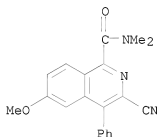
RN 849547-28-0 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxyethyl)-6-methoxy-4-phenyl-  
(CA INDEX NAME)



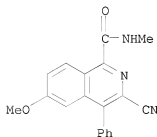
RN 849547-31-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N,N-dimethyl-4-phenyl- (CA  
INDEX NAME)



RN 849547-33-7 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-methyl-4-phenyl- (CA INDEX  
NAME)

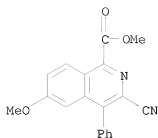


RN 849547-35-9 HCAPLUS

CN 1-Isoquinolinecarboxylic acid, 3-cyano-6-methoxy-4-phenyl-, methyl ester  
(CA INDEX NAME)

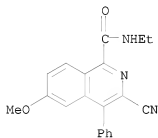
Updated Search

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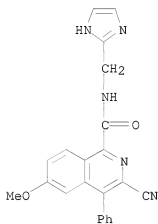
RN 849547-37-1 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-ethyl-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-39-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(1H-imidazol-2-ylmethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

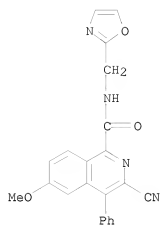


RN 849547-41-7 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-oxazolylmethyl)-4-phenyl- (CA INDEX NAME)

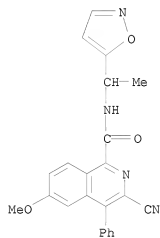
Updated Search

stn



RN 849547-43-9 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[1-(5-isoxazolyl)ethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

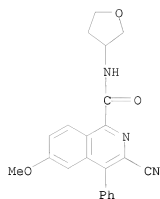


RN 849547-45-1 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(tetrahydro-3-furanyl)- (CA INDEX NAME)

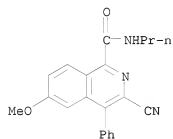
Updated Search

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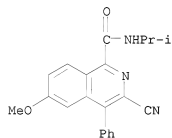
RN 849547-47-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-propyl- (CA INDEX NAME)



RN 849547-49-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(1-methylethyl)-4-phenyl- (CA INDEX NAME)



RN 849547-50-8 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(2-pyridinylmethyl)- (CA INDEX NAME)

Updated Search

1-Isoquinolinecarboxamide, 3-cyano-N-(2,3-dihydroxypropyl)-6-methoxy-4-

phenyl- (CA INDEX NAME)

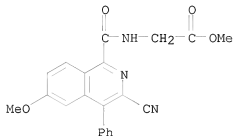
1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(tetrahydro-2-oxo-

3-furanyl)- (CA INDEX NAME)

stn

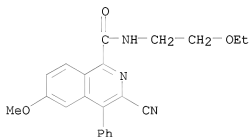
RN 849547-53-1 HCAPLUS

CN Glycine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]-, methyl ester (CA INDEX NAME)



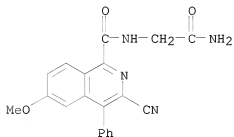
RN 849547-54-2 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-ethoxyethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-55-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, N-(2-amino-2-oxoethyl)-3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)

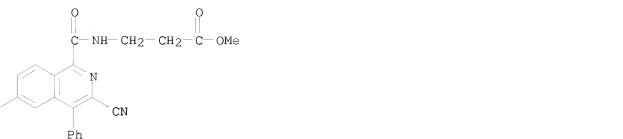


RN 849547-57-5 HCAPLUS

CN β-Alanine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]-, methyl ester (CA INDEX NAME)

Updated Search



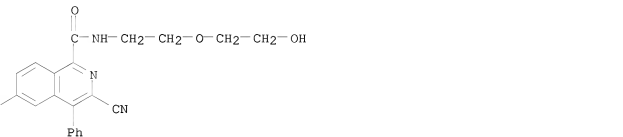


849547-59-7 HCAPLUS

1-Isoquinolinecarboxamide, 3-cyano-N-(3-hydroxypropyl)-6-methoxy-4-phenyl-  
(CA INDEX NAME)

849547-61-1 HCAPLUS

1-Isoquinolinecarboxamide, 3-cyano-N-[2-(2-hydroxyethoxy)ethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

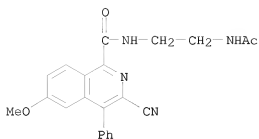


849547-63-3 HCAPLUS

1-Isoquinolinecarboxamide, N-[2-(acetylamino)ethyl]-3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)

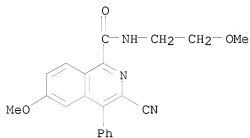
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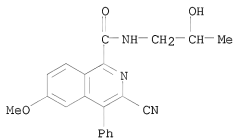
RN 849547-65-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-methoxyethyl)-4-phenyl-  
(CA INDEX NAME)



RN 849547-67-7 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxypropyl)-6-methoxy-4-phenyl-  
(CA INDEX NAME)

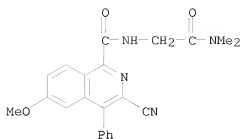


RN 849547-68-8 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[2-(dimethylamino)-2-oxoethyl]-6-methoxy-4-phenyl-  
(CA INDEX NAME)

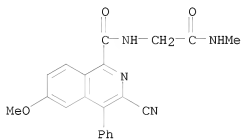
Updated Search

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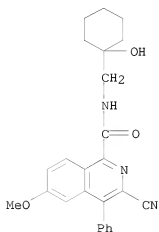
RN 849547-69-9 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-[2-(methylamino)-2-oxoethyl]-4-phenyl- (CA INDEX NAME)



RN 849547-71-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1-hydroxycyclohexyl)methyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

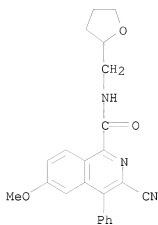


RN 849547-73-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[(tetrahydro-2-furanyl)methyl]- (CA INDEX NAME)

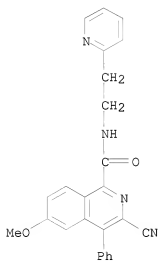
Updated Search

stn



RN 849547-75-7 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[2-(2-pyridinyl)ethyl]- (CA INDEX NAME)

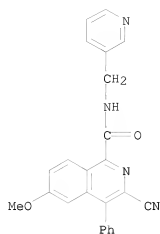


RN 849547-76-8 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(3-pyridinylmethyl)- (CA INDEX NAME)

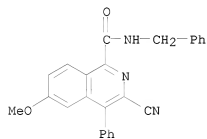
Updated Search

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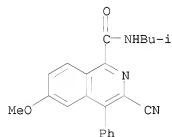
RN 849547-78-0 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(phenylmethyl)-  
(CA INDEX NAME)



RN 849547-80-4 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-methylpropyl)-4-phenyl-  
(CA INDEX NAME)

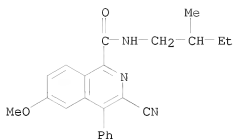


RN 849547-81-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-(2-methylbutyl)-4-phenyl-  
(CA INDEX NAME)

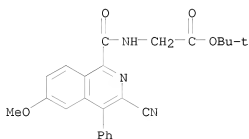
Updated Search

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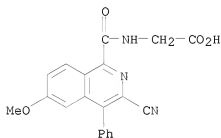
RN 849547-83-7 HCAPLUS

CN Glycine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 849547-85-9 HCAPLUS

CN Glycine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]- (CA INDEX NAME)

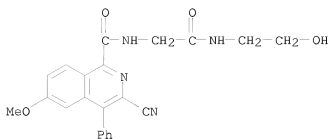


RN 849547-87-1 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[2-[(2-hydroxyethyl)amino]-2-oxoethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

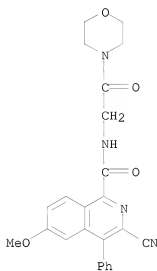
Updated Search

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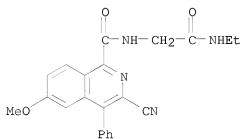
RN 849547-88-2 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-[2-(4-morpholinyl)-2-oxoethyl]-4-phenyl- (CA INDEX NAME)



RN 849547-90-6 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[2-(ethylamino)-2-oxoethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

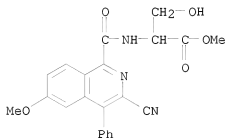


RN 849547-91-7 HCAPLUS

Updated Search

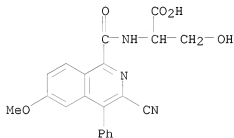
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CN Serine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]-, methyl ester (CA INDEX NAME)



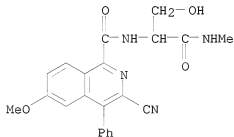
RN 849547-92-8 HCAPLUS

CN Serine, N-[(3-cyano-6-methoxy-4-phenyl-1-isoquinolinyl)carbonyl]- (CA INDEX NAME)



RN 849547-93-9 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[1-(hydroxymethyl)-2-(methylamino)-2-oxoethyl]-6-methoxy-4-phenyl- (CA INDEX NAME)



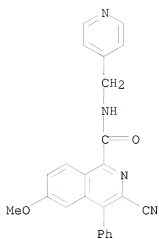
RN 849547-95-1 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-(4-pyridinylmethyl)- (CA INDEX NAME)

Updated Search

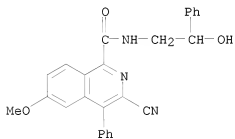


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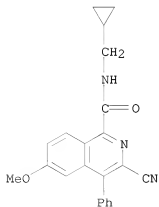
RN 849547-96-2 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-hydroxy-2-phenylethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849547-97-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(cyclopropylmethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



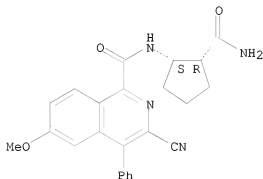
Updated Search

stn

RN 849547-99-5 HCAPLUS

CN 1-Isoquinolinecarboxamide, N-[(1S,2R)-2-(aminocarbonyl)cyclopentyl]-3-cyano-6-methoxy-4-phenyl- (CA INDEX NAME)

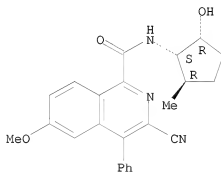
Absolute stereochemistry.



RN 849548-00-1 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1S,2R,5R)-2-hydroxy-5-methylcyclopentyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

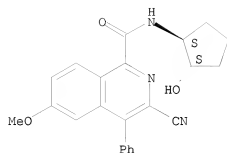


RN 849548-01-2 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1S,2S)-2-hydroxycyclopentyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

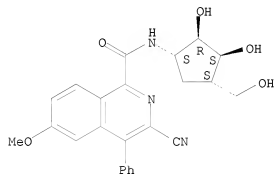
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RN 849548-02-3 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-[(1S,2R,3S,4S)-2,3-dihydroxy-4-(hydroxymethyl)cyclopentyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

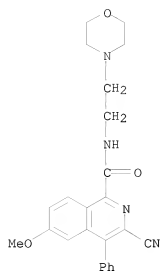


RN 849548-03-4 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-N-[2-(4-morpholinyl)ethyl]-4-phenyl- (CA INDEX NAME)

Updated Search

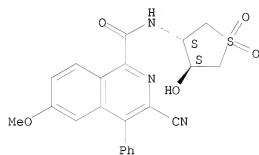
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RN 849548-04-5 HCAPLUS

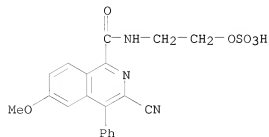
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[(3S,4S)-tetrahydro-4-hydroxy-1,1-dioxido-3-thienyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 849548-05-6 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[2-(sulfoxy)ethyl]- (CA INDEX NAME)



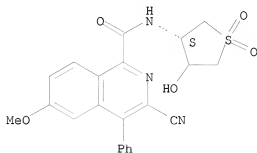
Updated Search

stn

RN 849548-06-7 HCAPLUS

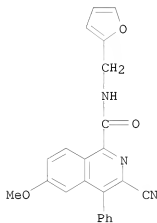
CN 1-Isoquinolinecarboxamide, 3-cyano-6-methoxy-4-phenyl-N-[(3S)-tetrahydro-4-hydroxy-1,1-dioxido-3-thienyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 849548-07-8 HCAPLUS

CN 1-Isoquinolinecarboxamide, 3-cyano-N-(2-furanylmethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

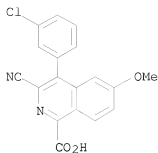


RN 849548-08-9 HCAPLUS

CN 1-Isoquinolinecarboxylic acid, 4-(3-chlorophenyl)-3-cyano-6-methoxy- (CA INDEX NAME)

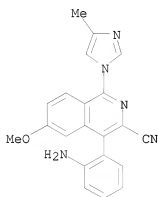
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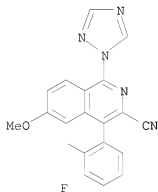
RN 849548-34-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(2-aminophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)



RN 849548-46-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(1H-1,2,4-triazol-1-yl)- (CA INDEX NAME)



RN 849548-47-6 HCAPLUS

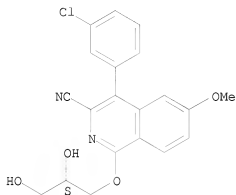
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[(2S)-2,3-

Updated Search

stn

dihydroxypropoxy]-6-methoxy- (CA INDEX NAME)

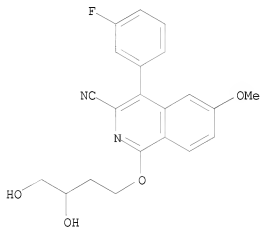
Absolute stereochemistry.



RN 849548-48-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(3,4-dihydroxybutoxy)-4-(3-fluorophenyl)-6-methoxy-, (+)- (CA INDEX NAME)

Rotation (+).



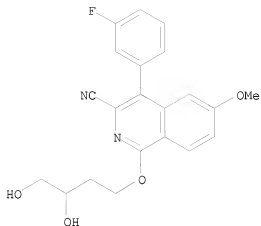
RN 849548-49-8 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(3,4-dihydroxybutoxy)-4-(3-fluorophenyl)-6-methoxy-, (-)- (CA INDEX NAME)

Rotation (-).

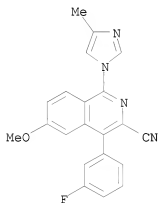
Updated Search

stn



RN 849548-50-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)



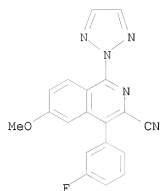
RN 849548-51-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(2H-1,2,3-triazol-2-yl)- (CA INDEX NAME)

Updated Search

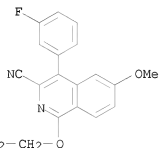


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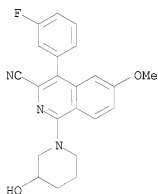
RN 849548-52-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-[2-[(2-hydroxyethyl)amino]ethoxy]-6-methoxy- (CA INDEX NAME)



RN 849548-53-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-1-(3-hydroxy-1-piperidinyl)-6-methoxy- (CA INDEX NAME)

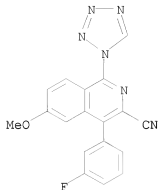


RN 849548-54-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(1H-tetrazol-1-yl)- (CA INDEX NAME)

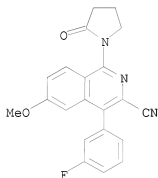
Updated Search

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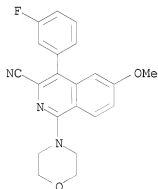
RN 849548-55-6 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(2-oxo-1-pyrrolidinyl)- (CA INDEX NAME)



RN 849548-56-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-fluorophenyl)-6-methoxy-1-(4-morpholinyl)- (CA INDEX NAME)

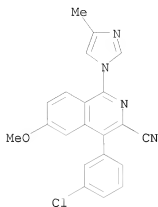


RN 849548-57-8 HCAPLUS

Updated Search

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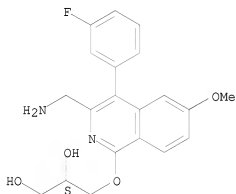
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-(4-methyl-1H-imidazol-1-yl)- (CA INDEX NAME)



RN 849548-58-9 HCAPLUS

CN 1,2-Propanediol, 3-[[3-(aminomethyl)-4-(3-fluorophenyl)-6-methoxy-1-isoquinolinyl]loxy]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

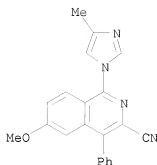


RN 849548-59-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(4-methyl-1H-imidazol-1-yl)-4-phenyl- (CA INDEX NAME)

Updated Search

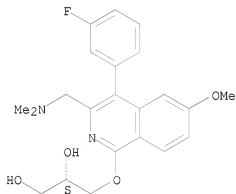
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RN 849548-60-3 HCAPLUS

CN 1,2-Propanediol, 3-[[3-[(dimethylamino)methyl]-4-(3-fluorophenyl)-6-methoxy-1-isoquinolinyloxy]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

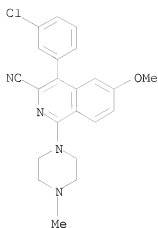


RN 849548-61-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-(4-methyl-1-piperazinyl)- (CA INDEX NAME)

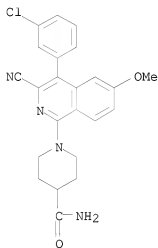
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RN 849548-64-7 HCAPLUS

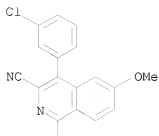
CN 4-Piperidinecarboxamide, 1-[4-(3-chlorophenyl)-3-cyano-6-methoxy-1-isoquinolinyl]- (CA INDEX NAME)



RN 849548-65-8 HCAPLUS

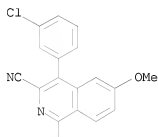
CN 3-Isoquinolinecarbonitrile, 1-[(3-aminopropyl)amino]-4-(3-chlorophenyl)-6-methoxy- (CA INDEX NAME)

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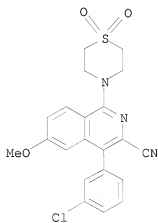
RN 849548-66-9 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2-aminoethyl)amino]-4-(3-chlorophenyl)-6-methoxy- (CA INDEX NAME)



RN 849548-67-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-(1,1-dioxido-4-thiomorpholinyl)-6-methoxy- (CA INDEX NAME)

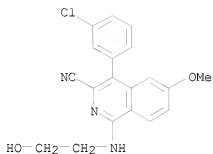


RN 849548-68-1 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[(2-hydroxyethyl)amino]-6-methoxy- (CA INDEX NAME)

Updated Search

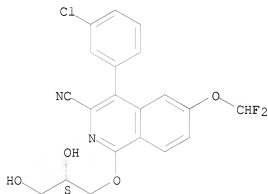
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RN 849548-69-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-(difluoromethoxy)-1-[(2S)-2,3-dihydroxypropoxy]- (CA INDEX NAME)

Absolute stereochemistry.

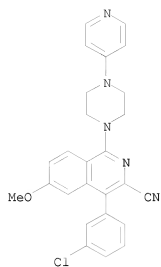


RN 849548-70-5 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-[4-(4-pyridinyl)-1-piperazinyl]- (CA INDEX NAME)

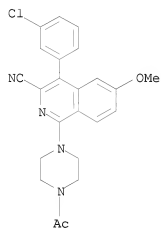
Updated Search

stn



RN 849548-71-6 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-(4-(3-chlorophenyl)-4-(3-pyridinyl)-6-methoxy- (CA INDEX NAME)



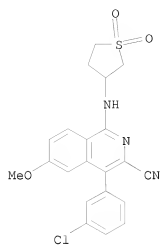
RN 849548-72-7 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-6-methoxy-1-[(tetrahydro-1,1-dioxido-3-thienyl)amino]- (CA INDEX NAME)

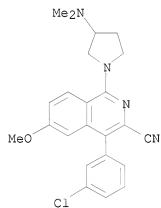
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stn



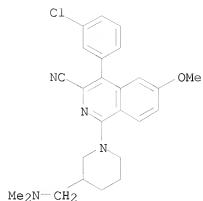
RN 849548-73-8 HCAPLUS  
CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[3-(dimethylamino)-1-pyrrolidinyl]-6-methoxy- (CA INDEX NAME)



RN 849548-74-9 HCAPLUS  
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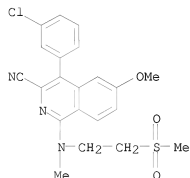
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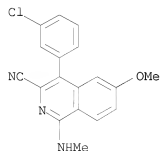
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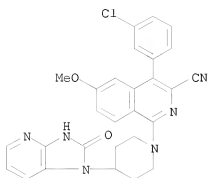


RN 849548-77-2 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 4-(3-chlorophenyl)-1-[4-(2,3-dihydro-2-oxo-1H-imidazo[4,5-b]pyridin-1-yl)-1-piperidinyl]-6-methoxy- (CA INDEX NAME)

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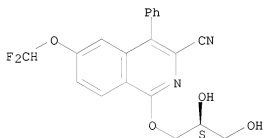
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RN 849548-78-3 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-(difluoromethoxy)-1-[(2S)-2,3-dihydroxypropoxy]-4-phenyl- (CA INDEX NAME)

Absolute stereochemistry.

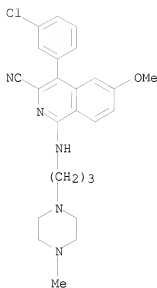


RN 849548-79-4 HCAPLUS

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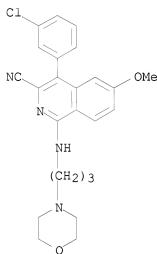
Updated Search

stn



RN 849548-80-7 HCAPLUS

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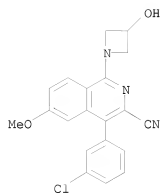


RN 849548-81-8 HCAPLUS

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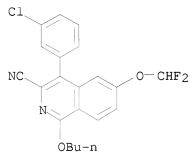
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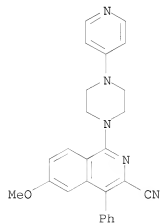
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RN 849548-83-0 HCAPLUS

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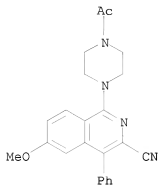


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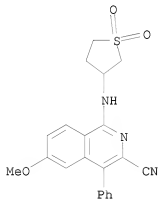
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(CA INDEX NAME)



RN 849548-85-2 HCAPLUS

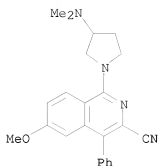
CN 3-Isoquinolinecarbonitrile, 6-methoxy-4-phenyl-1-[(tetrahydro-1,1-dioxido-3-thienyl)amino]- (CA INDEX NAME)



RN 849548-86-3 HCAPLUS

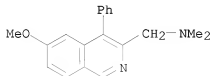
CN 3-Isoquinolinecarbonitrile, 1-[3-(dimethylamino)-1-pyrrolidinyl]-6-methoxy-4-phenyl- (CA INDEX NAME)

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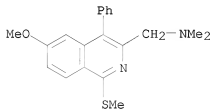
RN 849549-04-8 HCAPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-4-phenyl- (CA INDEX NAME)



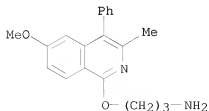
RN 849549-05-9 HCAPLUS

CN 3-Isoquinolinemethanamine, 6-methoxy-N,N-dimethyl-1-(methylthio)-4-phenyl- (CA INDEX NAME)



RN 849549-06-0 HCAPLUS

CN 1-Propanamine, 3-[(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)oxy]- (CA INDEX NAME)

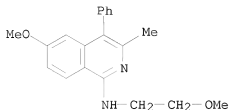


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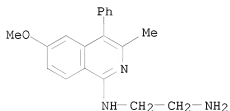
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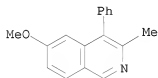
RN 849549-08-2 HCAPLUS

CN 1,2-Ethanediamine, N1-(6-methoxy-3-methyl-4-phenyl-1-isoquinolinyl)- (CA INDEX NAME)



RN 849549-09-3 HCAPLUS

CN Isoquinoline, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)

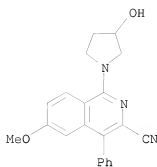


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CN 3-Isoquinolinecarbonitrile, 1-(3-hydroxy-1-pyrrolidinyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



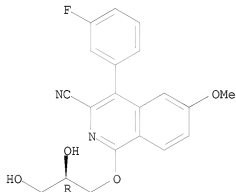
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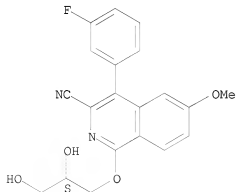
Absolute stereochemistry.



RN 849549-12-8 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[(2S)-2,3-dihydroxypropoxy]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



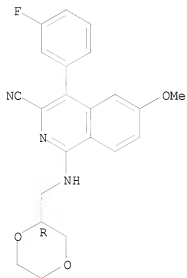
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RN 849549-13-9 HCAPLUS

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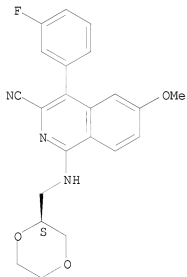
Absolute stereochemistry.



RN 849549-14-0 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[ (2S)-1,4-dioxan-2-ylmethyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



RN 849549-15-1 HCAPLUS

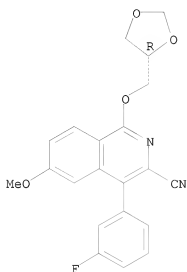
CN 3-Isoquinolinecarbonitrile, 1-[(4R)-1,3-dioxolan-4-ylmethoxy]-4-(3-

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fluorophenyl)-6-methoxy- (CA INDEX NAME)

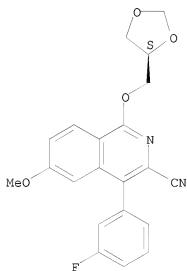
Absolute stereochemistry.



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Absolute stereochemistry.

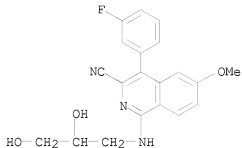


RN 849549-17-3 HCAPLUS

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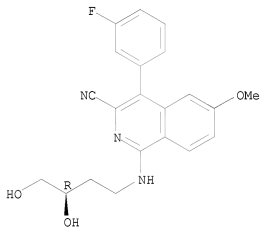
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RN 849549-18-4 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[ (3R)-3,4-dihydroxybutyl]amino]-4-(3-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.

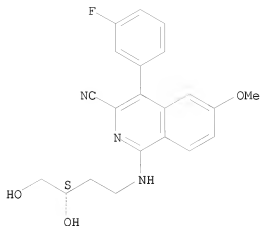


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Absolute stereochemistry.

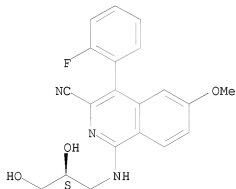
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RN 849549-20-8 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 1-[[ (2S)-2,3-dihydroxypropyl]amino]-4-(2-fluorophenyl)-6-methoxy- (CA INDEX NAME)

Absolute stereochemistry.



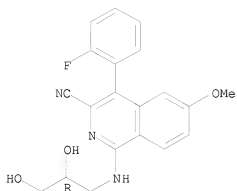
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Absolute stereochemistry.

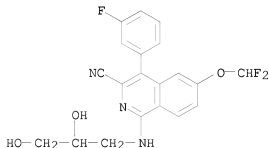
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RN 849549-22-0 HCAPLUS

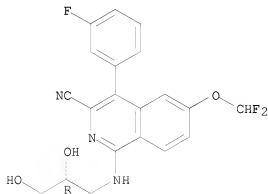
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RN 849549-23-1 HCAPLUS

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Absolute stereochemistry.



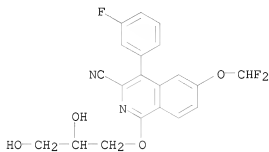
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Updated Search

stn

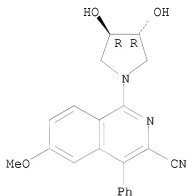
(3-fluorophenyl)- (CA INDEX NAME)



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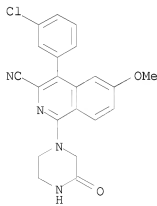
CN 3-Isoquinolinecarbonitrile, 1-[(3R,4R)-3,4-dihydroxy-1-pyrrolidinyl]-6-methoxy-4-phenyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 849549-32-2 HCAPLUS

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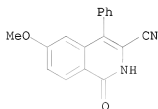
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IT 849549-26-4 849549-27-5 849549-29-7  
849635-33-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of isoquinoline derivs. as potassium channel inhibitors)

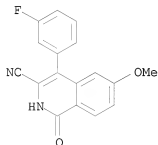
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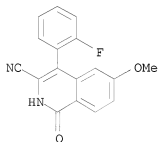
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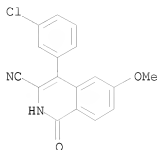
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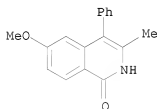
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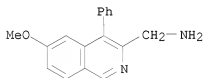
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 849548-93-2P 849548-94-3P 849548-97-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of isoquinoline derivs. as potassium channel inhibitors)  
 RN 849424-95-9 HCAPLUS  
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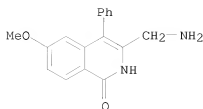
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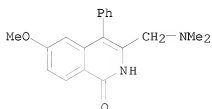
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Updated Search

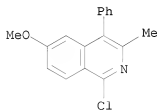
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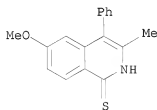
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CN 1(2H)-Isoquinolinone, 3-[(dimethylamino)methyl]-6-methoxy-4-phenyl- (CA INDEX NAME)



RN 849548-90-9 HCAPLUS  
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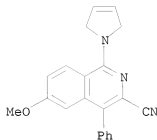
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CN 1(2H)-Isoquinolinethione, 6-methoxy-3-methyl-4-phenyl- (CA INDEX NAME)



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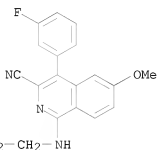
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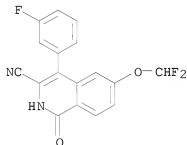
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RN 849548-97-6 HCAPLUS

CN 3-Isoquinolinecarbonitrile, 6-(difluoromethoxy)-4-(3-fluorophenyl)-1,2-dihydro-1-oxo- (CA INDEX NAME)



=> d his

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FILE 'REGISTRY' ENTERED AT 06:01:29 ON 08 DEC 2008

L1 STRUCTURE UPLOADED

Updated Search

stn

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L3 277 S L1 FULL

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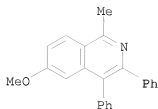
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L6 ANSWER 1 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN  
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TITLE: Chlorotris(triphenylphosphine)-rhodium(I)  
AUTHOR(S): Burgess, Kevin; van der Donk, Wilfred A.  
CORPORATE SOURCE: USA  
SOURCE: e-EROS Encyclopedia of Reagents for Organic Synthesis  
(2001), No pp. given. John Wiley & Sons, Ltd.:  
Chichester, UK.  
CODEN: 69KUHI  
URL: <http://www3.interscience.wiley.com/cgi-bin/mrw/home/104554785/HOME>  
DOCUMENT TYPE: Conference; General Review; (online computer file)  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 149:307083  
AB A review of the article Chlorotris(triphenylphosphine)-rhodium(I).  
IT 585531-20-0P 585531-23-3P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(Chlorotris(triphenylphosphine)-rhodium(I))  
RN 585531-20-0 HCAPLUS  
CN Isoquinoline, 6-methoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)

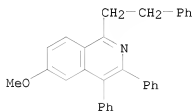
Updated Search

stn



RN 585531-23-3 HCAPLUS

CN Isoquinoline, 6-methoxy-3,4-diphenyl-1-(2-phenylethyl)- (CA INDEX NAME)



L6 ANSWER 2 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:1043244 HCAPLUS

DOCUMENT NUMBER: 145:454923

TITLE: A convenient synthesis of 1,4-disubstituted isoquinolines by reactions of  $\alpha$ -substituted 2-lithio- $\beta$ -methoxystyrenes with nitriles

AUTHOR(S): Kobayashi, Kazuhiro; Hayashi, Kazutaka; Miyamoto,

Kazuna; Morikawa, Osamu; Konishi, Hisatoshi

CORPORATE SOURCE: Department of Materials Science, Faculty of Engineering, Tottori University, 4-101 Koyama-minami, Tottori, 680-8552, Japan

SOURCE: Synthesis (2006), (17), 2934-2938

CODEN: SYNTBF; ISSN: 0039-7881

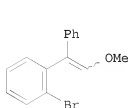
PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

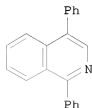
LANGUAGE: English

OTHER SOURCE(S): CASREACT 145:454923

GI



I



II

Updated Search

stn

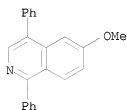
AB It has been found that halogen-lithium exchange between  $\alpha$ -substituted 2-bromo- $\beta$ -methoxystyrene derivs., e.g., I, and n-butyllithium generates  $\alpha$ -substituted 2-lithio- $\beta$ -methoxystyrene derivs., which successfully react with a range of nitriles to afford the corresponding 1,4-disubstituted isoquinolines, e.g., II, in reasonable yields.

IT 82894-69-7P 913192-02-6P 913192-03-7P  
913192-04-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of disubstituted isoquinolines by halogen lithium exchange of bromomethoxystyrenes with n-butyllithium and subsequent condensation with aryl/alkyl nitriles)

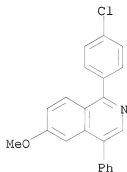
RN 82894-69-7 HCAPLUS

CN Isoquinoline, 6-methoxy-1,4-diphenyl- (CA INDEX NAME)



RN 913192-02-6 HCAPLUS

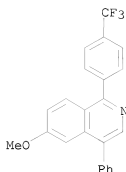
CN Isoquinoline, 1-(4-chlorophenyl)-6-methoxy-4-phenyl- (CA INDEX NAME)



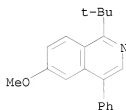
RN 913192-03-7 HCAPLUS

CN Isoquinoline, 6-methoxy-4-phenyl-1-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)

stn



RN 913192-04-8 HCAPLUS  
CN Isoquinoline, 1-(1,1-dimethylethyl)-6-methoxy-4-phenyl- (CA INDEX NAME)

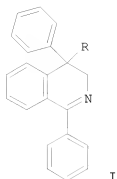


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2006:764380 HCAPLUS  
DOCUMENT NUMBER: 145:377169  
TITLE: New synthesis of isoquinoline and  
3,4-dihydroisoquinoline derivatives  
AUTHOR(S): Kobayashi, Kazuhiro; Shiokawa, Taiyo; Omote, Hiroki;  
Hashimoto, Kenichi; Morikawa, Osamu; Konishi,  
Hisatoshi  
CORPORATE SOURCE: Department of Materials Science, Faculty of  
Engineering, Tottori University, 4-101 Koyama-minami,  
Tottori, 680-8552, Japan  
SOURCE: Bulletin of the Chemical Society of Japan (2006),  
79(7), 1126-1132  
CODEN: BCSJA8; ISSN: 0009-2673  
PUBLISHER: Chemical Society of Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 145:377169  
GI

Updated Search

stn



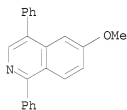
AB A simple and efficient synthesis of isoquinoline and 3,4-dihydroisoquinoline derivs. was described. 1-Alkyl(or aryl)isoquinoline and 1-isoquinolinamine derivs. were obtained by intramol. cyclization of 2-(2-methoxyethenyl)benzonitriles initiated by the addition of alkyl(or aryl)lithiums and lithium dialkylamides to the nitrile carbons, resp. Synthesis of 4-aryl-3,4-dihydroisoquinolines was achieved by reactions of 2-(1-arylethenyl)benzonitriles with organolithiums, followed by aqueous workup. Treatment of the reaction mixts. with electrophiles prior to aqueous workup allowed the synthesis of 4,4-disubstituted 3,4-dihydroisoquinolines, e.g., I (Me, Et, Bn or t-BuOCOCH<sub>2</sub>).

IT 82894-69-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of alkyl- or (aryl)isoquinoline derivs. via intramol. heterocyclization of (methoxyethenyl)benzonitriles initiated by addition of alkyl- or (aryl)lithiums to nitrile carbons)

RN 82894-69-7 HCAPLUS

CN Isoquinoline, 6-methoxy-1,4-diphenyl- (CA INDEX NAME)



IT 686719-45-9P

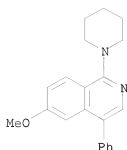
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of isoquinolinamine derivs. via intramol. heterocyclization of (methoxyethenyl)benzonitriles initiated by the addition of lithium dialkylamides to nitrile carbons)

RN 686719-45-9 HCAPLUS

CN Isoquinoline, 6-methoxy-4-phenyl-1-(1-piperidinyl)- (CA INDEX NAME)



stn



REFERENCE COUNT: 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:1007173 HCAPLUS

DOCUMENT NUMBER: 143:440242

TITLE: Novel Methods for the Synthesis of 4-Arylisoquinolinium Perchlorates and 4-Arylisoquinolin-1-ones

AUTHOR(S): Coskun, Necdet; Kizilkusak, Yunus  
CORPORATE SOURCE: Department of Chemistry, Uludag University, Goeruekle Bursa, Turk.

SOURCE: Synthetic Communications (2005), 35(18), 2435-2443

CODEN: SYNCV; ISSN: 0039-7911

PUBLISHER: Taylor & Francis, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 143:440242

AB 2-Benzylamino-1-phenylethanones were converted to the corresponding isoquinolinium perchlorates (I) in high yields using 70% HClO<sub>4</sub>-FeCl<sub>3</sub> mixture as a cyclization and oxidation reagent. A mild and high yielding method for the subsequent oxidation of I to isoquinolin-1-ones involving the treatment of I with KOH and K<sub>3</sub>[Fe(CN)<sub>6</sub>] in THF-H<sub>2</sub>O two-phase system at room temperature was developed. Compds. I disproportionate to isoquinolin-1-ones and the corresponding 1,2-dihydroisoquinoline in the presence of base, which in turn is oxidized by K<sub>3</sub>[Fe(CN)<sub>6</sub>] to I.

IT 206126-10-5P 868601-73-4P 868601-75-6P

868601-78-9P 868601-80-3P 868601-84-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of arylisoquinolinium perchlorates and arylisoquinolinones from (benzylamino)phenylethanones by cyclization and oxidation)

RN 206126-10-5 HCAPLUS

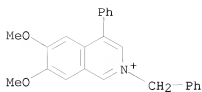
CN Isoquinolinium, 6,7-dimethoxy-4-phenyl-2-(phenylmethyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 206126-09-2

CMF C24 H22 N O2

stn



CM 2

CRN 14797-73-0

CMF C1 O4



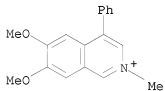
RN 868601-73-4 HCAPLUS

CN Isoquinolinium, 6,7-dimethoxy-2-methyl-4-phenyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 868601-72-3

CMF C18 H18 N O2



CM 2

CRN 14797-73-0

CMF C1 O4



RN 868601-75-6 HCAPLUS

CN Isoquinolinium, 2-ethyl-6,7-dimethoxy-4-phenyl-, perchlorate (1:1) (CA

Updated Search

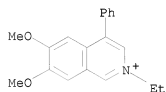
stn

INDEX NAME)

CM 1

CRN 868601-74-5

CMF C19 H20 N O2



CM 2

CRN 14797-73-0

CMF C1 O4



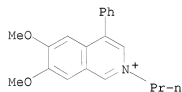
RN 868601-78-9 HCAPLUS

CN Isoquinolinium, 6,7-dimethoxy-4-phenyl-2-propyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 868601-77-8

CMF C20 H22 N O2



CM 2

CRN 14797-73-0

CMF C1 O4

Updated Search

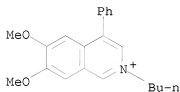
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RN 868601-80-3 HCAPLUS  
CN Isoquinolinium, 2-butyl-6,7-dimethoxy-4-phenyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 868601-79-0  
CMF C21 H24 N O2



CM 2

CRN 14797-73-0  
CMF Cl O4



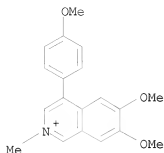
RN 868601-84-7 HCAPLUS  
CN Isoquinolinium, 6,7-dimethoxy-4-(4-methoxyphenyl)-2-methyl-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 868601-83-6  
CMF C19 H20 N O3

Updated Search

stn



CM 2

CRN 14797-73-0

CMF C1 O4



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:408217 HCAPLUS  
Correction of: 2005:155220

DOCUMENT NUMBER: 143:266757  
Correction of: 142:197771

TITLE: Product class 5: isoquinolines

AUTHOR(S): Alvarez, M.; Joule, J. A.

CORPORATE SOURCE: Germany

SOURCE: Science of Synthesis (2005), 15, 661-838

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review primarily covering methods of preparation of isoquinolines via cyclization, ring transformations or substituent modification.

Isoquinoline 2-oxides and isoquinolinium salts are also included.

IT 585531-20-0P 585531-23-3P

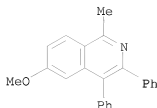
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of isoquinolines and analogs via cyclization, ring transformations or substituent modifications)

RN 585531-20-0 HCAPLUS

CN Isoquinoline, 6-methoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)

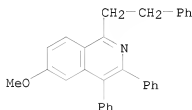
Updated Search

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RN 585531-23-3 HCAPLUS

CN Isoquinoline, 6-methoxy-3,4-diphenyl-1-(2-phenylethyl)- (CA INDEX NAME)



L6 ANSWER 6 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:248544 HCAPLUS

DOCUMENT NUMBER: 142:482016

TITLE: Direct, Two-Step Synthetic Pathway to Novel Dibenzo[a,c]phenanthridines

AUTHOR(S): Churrua, Fatima; SanMartin, Raul; Carril, Monica; Urtiaga, Miren Karmele; Solans, Xavier; Tellitu, Imanol; Dominguez, Esther

CORPORATE SOURCE: Kimika Organikoa II Saila, Zientzi eta Teknologia Fakultatea, Euskal Herriko Unibertsitatea, Bilbao, 48080, Spain

SOURCE: Journal of Organic Chemistry (2005), 70(8), 3178-3187  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:482016

AB Novel dibenzo[a,c]phenanthridines are prepared regioselectively by the application of a straightforward synthetic pathway, starting from new 3,4-diaryl- and 3,4-dihydro-3,4-diarylisquinolines prepared via Ritter-type heterocyclization and the more classical two-step reductive amination/Bischler-Napieralski cyclization of triarylethanones, resp. A comparative study of nonphenolic oxidative coupling methodologies provides a highly efficient procedure, based on the hypervalent iodine reagent phenyliodine(III) bis(trifluoroacetate) (PIFA), to accomplish the final coupling step.

IT 851962-30-6P 851962-31-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

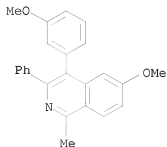
(preparation of 3,4-diaryl- and 3,4-dihydro-3,4-diarylisquinolines via Ritter-type heterocyclization of triarylethanones)

RN 851962-30-6 HCAPLUS

Updated Search

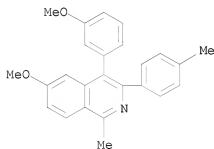
stn

CN Isoquinoline, 6-methoxy-4-(3-methoxyphenyl)-1-methyl-3-phenyl- (CA INDEX NAME)



RN 851962-31-7 HCAPLUS

CN Isoquinoline, 6-methoxy-4-(3-methoxyphenyl)-1-methyl-3-(4-methylphenyl)- (CA INDEX NAME)



IT 851962-23-7P 851962-24-8P 851962-25-9P

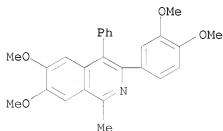
851962-26-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(two-step synthetic pathway to dibenzo[a,c]phenanthridines based on ketone heterocyclization and oxidative biaryl coupling)

RN 851962-23-7 HCAPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-4-phenyl- (CA INDEX NAME)

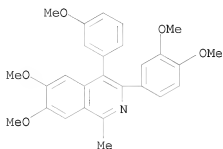


RN 851962-24-8 HCAPLUS

Updated Search

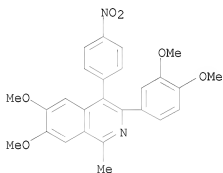
stn

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-4-(3-methoxyphenyl)-1-methyl- (CA INDEX NAME)



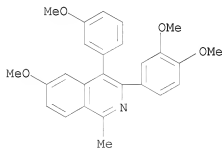
RN 851962-25-9 HCAPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-4-(4-nitrophenyl)- (CA INDEX NAME)



RN 851962-26-0 HCAPLUS

CN Isoquinoline, 3-(3,4-dimethoxyphenyl)-6-methoxy-4-(3-methoxyphenyl)-1-methyl- (CA INDEX NAME)



REFERENCE COUNT:

106

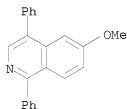
THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

Updated Search

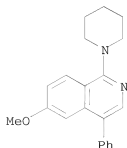


stn

L6 ANSWER 7 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2004:231365 HCAPLUS  
DOCUMENT NUMBER: 140:391184  
TITLE: New synthesis of isoquinoline derivatives by reactions  
of 2-(2-methoxyethenyl)benzonitriles with  
organolithiums and lithium dialkylamides  
AUTHOR(S): Kobayashi, Kazuhiro; Shiokawa, Taiyo; Morikawa, Osamu;  
Konishi, Hisatoshi  
CORPORATE SOURCE: Department of Materials Science, Faculty of  
Engineering, Tottori University, Tottori, 680-8552,  
Japan  
SOURCE: Chemistry Letters (2004), 33(3), 236-237  
CODEN: CMLTAG; ISSN: 0366-7022  
PUBLISHER: Chemical Society of Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 140:391184  
AB A simple and efficient synthesis of 1-alkyl(or aryl)isoquinoline and  
isoquinolin-1-amine derivs. based on intramol. cyclization of  
2-(2-methoxyethenyl)benzonitriles initiated by the addition of alkyl(or  
aryl)lithiums and lithium dialkylamides to the nitrile carbons, resp., is  
described.  
IT 82894-69-7P 686719-45-9P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of isoquinoline derivs. by intramol. cyclization of  
2-(2-methoxyethenyl)benzonitriles with organolithiums and lithium  
dialkylamides)  
RN 82894-69-7 HCAPLUS  
CN Isoquinoline, 6-methoxy-1,4-diphenyl- (CA INDEX NAME)



RN 686719-45-9 HCAPLUS  
CN Isoquinoline, 6-methoxy-4-phenyl-1-(1-piperidinyl)- (CA INDEX NAME)



Updated Search

stn

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:505035 HCAPLUS

DOCUMENT NUMBER: 139:197350

TITLE: Rh(I)-Catalyzed Direct ortho-Alkenylation of Aromatic Ketimines with Alkynes and its Application to the Synthesis of Isoquinoline Derivatives

AUTHOR(S): Lim, Sung-Gon; Lee, Jun Hee; Moon, Choong Woon; Hong, Jun-Bae; Jun, Chul-Ho

CORPORATE SOURCE: Department of Chemistry, Yonsei University, Seoul, 120-749, S. Korea

SOURCE: Organic Letters (2003), 5(15), 2759-2761

CODEN: ORLEF7; ISSN: 1523-7060

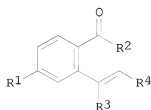
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

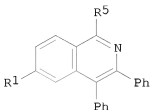
LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:197350

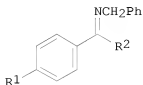
GI



I



II



III

AB Novel synthetic methods for preparation of both ortho-alkenylated aromatic ketones

I (R<sup>1</sup> = H, F3C, MeO; R<sup>2</sup> = Me, Et, n-pentyl; R<sup>3</sup> = H, R<sup>4</sup> = Bu, Me3C, n-hexyl; R<sup>3</sup> = R<sup>4</sup> = Ph) and isoquinolines II (R<sup>5</sup> = Me, PhCH<sub>2</sub>CH<sub>2</sub>) have been developed via the Rh(I)-catalyzed direct ortho-alkenylation of common aromatic ketimines III with alkynes R<sup>3</sup>C.tplbond.CR<sup>4</sup>. Furthermore, a highly efficient one-pot synthesis of isoquinolines II was achieved by simply mixing aromatic ketone 4-R<sup>1</sup>C<sub>6</sub>H<sub>4</sub>COMe, benzylamine, and diphenylacetylene in the presence of a Rh(I) catalyst.

IT 585531-20-0P 585531-23-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

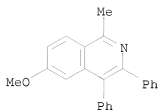
(preparation of alkenylphenyl ketones, alkenylphenyl ketimines and isoquinolines via Rh(I)-catalyzed direct ortho-alkenylation of aromatic ketimines with alkynes)

RN 585531-20-0 HCAPLUS

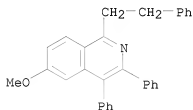
CN Isoquinoline, 6-methoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)

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RN 585531-23-3 HCAPLUS  
CN Isoquinoline, 6-methoxy-3,4-diphenyl-1-(2-phenylethyl)- (CA INDEX NAME)



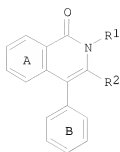
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2002:902258 HCAPLUS  
DOCUMENT NUMBER: 137:379992  
TITLE: Method of inhibiting neoplastic cells with  
isoquinolinonecarboxylates  
INVENTOR(S): Pamukcu, Rifat; Piazza, Gary A.  
PATENT ASSIGNEE(S): Cell Pathways, Inc., USA  
SOURCE: U.S., 119 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6486155	B1	20021126	US 1998-198413	19981124
PRIORITY APPLN. INFO.:			US 1998-198413	19981124
OTHER SOURCE(S):	MARPAT	137:379992		
GI				

Updated Search

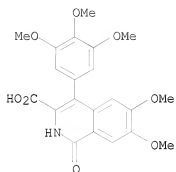
stn



I

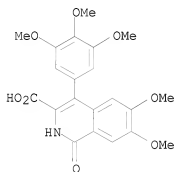
- AB A method is claimed for inhibiting neoplasia (no data), particularly cancerous and precancerous lesions, by exposing the affected cells to 1-isoquinoline-3-carboxylates. Such compds. are effective in modulating apoptosis and eliminating and inhibiting the growth of neoplasias such as precancerous lesions, but are not characterized by the severe side reactions of conventional non-steroidal antiinflammatory drugs or other chemotherapeutics. Although the methods of preparation are not claimed, example preps. of 429 isoquinolines and 107 intermediates are included; these examples are referenced to PCT application WO 98/38168. Although the claims indicate I (ring A and ring B are the same or different and each a (un)substituted benzene ring, R1 is morpholine, R2 is -COOR3, and R3 is alkyl; e.g. 7-benzyloxy-6-methoxy-3-methoxycarbonyl-2-morpholino-4-(3,4,5-trimethoxyphenyl)-1(2H)-isoquinolinone) or pharmaceutically acceptable salt thereof, the examples include a much broader variety of 1-isoquinoline-3-carboxylates.
- IT 212489-07-1P, 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-  
212489-10-6P, 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, monosodium salt 212489-49-1P, 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester 212500-07-7P, 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo-  
212500-10-2P, 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo-, methyl ester  
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of isoquinolinonecarboxylates for inhibiting neoplastic cells)
- RN 212489-07-1 HCAPLUS
- CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

stn



RN 212489-10-6 HCAPLUS

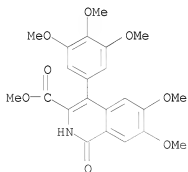
CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, sodium salt (1:1) (CA INDEX NAME)



● Na

RN 212489-49-1 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)

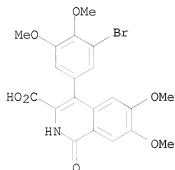


Updated Search

stn

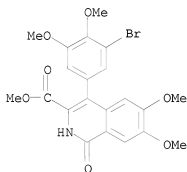
RN 212500-07-7 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo- (CA INDEX NAME)



RN 212500-10-2 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 171 THERE ARE 171 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L6 ANSWER 10 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:795461 HCAPLUS

DOCUMENT NUMBER: 136:69724

TITLE: Synthesis of Isoquinolines and Pyridines by the Palladium-Catalyzed Iminoannulation of Internal Alkynes

AUTHOR(S): Roesch, Kevin R.; Zhang, Haiming; Larock, Richard C.  
CORPORATE SOURCE: Department of Chemistry, Iowa State University, Ames, IA, 50011, USA

SOURCE: Journal of Organic Chemistry (2001), 66(24), 8042-8051  
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

Updated Search

stn

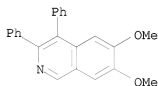
OTHER SOURCE(S): CASREACT 136:69724

AB A wide variety of substituted isoquinoline, tetrahydroisoquinoline, 5,6-dihydrobenz[f]isoquinoline, pyridine, and pyridine heterocycles have been prepared in good to excellent yields via annulation of internal acetylenes with the tert-butyldimines of o-iodobenzaldehydes and 3-halo-2-alkenals in the presence of a palladium catalyst. The best results are obtained by employing 5 mol % of Pd(OAc)<sub>2</sub>, an excess of the alkyne, 1 equiv of Na<sub>2</sub>CO<sub>3</sub> as a base, and 10 mol % of PPh<sub>3</sub> in DMF as the solvent. This annulation methodol. is particularly effective for aryl- or alkenyl-substituted alkynes. When electron-rich imines are employed, this chemical can be extended to alkyl-substituted alkynes. Trimethylsilyl-substituted alkynes also undergo this annulation process to afford monosubstituted heterocyclic products absent the silyl group.

IT 385416-24-0P 385416-26-2P 385416-28-4P  
385416-39-7P 385416-42-2P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of isoquinolines and pyridines by palladium-catalyzed iminoannulation of internal alkynes)

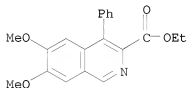
RN 385416-24-0 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-3,4-diphenyl- (CA INDEX NAME)



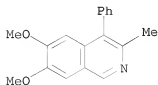
RN 385416-26-2 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-4-phenyl-, ethyl ester (CA INDEX NAME)



RN 385416-28-4 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-3-methyl-4-phenyl- (CA INDEX NAME)

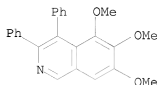


RN 385416-39-7 HCAPLUS

Updated Search

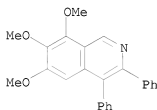
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CN Isoquinoline, 5,6,7-trimethoxy-3,4-diphenyl- (CA INDEX NAME)



RN 385416-42-2 HCAPLUS

CN Isoquinoline, 6,7,8-trimethoxy-3,4-diphenyl- (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:658540 HCAPLUS

DOCUMENT NUMBER: 135:371618

TITLE: Isoquinoline syntheses via  $\Delta^2$ -oxazolines. Part VIII. Cyclization of 2-acetamido-1,2-diphenylethan-1-ol derivatives into isoquinoline systems

AUTHOR(S): Kopczynski, T.; Voelkel, A.

CORPORATE SOURCE: Institute of Chemical Technology and Engineering, Poznan Technical University, Poznan, 60-965, Pol.  
SOURCE: Polish Journal of Chemistry (2001), 75(9), 1317-1325  
CODEN: PJCHDQ; ISSN: 0137-5083

PUBLISHER: Polish Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:371618

AB The results of the conversion of 2-acetamido-1,2-diphenylethan-1-ol derivs. into 1-methyl-4-phenylisoquinoline derivs. were described. The mechanism proposed for these reaction assumes the existence of protonated  $\Delta^2$ -oxazolines, carbonium ions, and unsatd. amides as intermediates. For example, the cyclization of erythro-N-(2-hydroxy-1,2-diphenylethyl)acetamide or threo-N-(2-hydroxy-1,2-diphenylethyl)acetamide gave 1-methyl-4-phenylisoquinoline in 66% yield.

IT 374594-09-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of isoquinolines via cyclocondensation of N-(hydroxydiphenylethyl)acetamide derivs.)

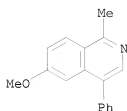
RN 374594-09-9 HCAPLUS

Updated Search



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CN Isoquinoline, 6-methoxy-1-methyl-4-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:355514 HCAPLUS

DOCUMENT NUMBER: 135:76771

TITLE: Novel, potent, and selective phosphodiesterase 5 inhibitors: synthesis and biological activities of a series of 4-aryl-1-isoquinolinone derivatives  
AUTHOR(S): Ukita, Tatsuzo; Nakamura, Yoshinori; Kubo, Akira; Yamamoto, Yasuo; Moritani, Yasunori; Saruta, Kunio; Higashijima, Takanori; Kotera, Jun; Takagi, Michino; Kikkawa, Kohei; Omori, Kenji

CORPORATE SOURCE: Discovery Research Laboratory, Tanabe Seiyaku Co. Ltd., Yodogawa Osaka, 532-8505, Japan

SOURCE: Journal of Medicinal Chemistry (2001), 44(13), 2204-2218

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:76771

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A novel class of potent and selective phosphodiesterase 5 (PDE5) inhibitors, the hydrochlorides of 4-aryl-1-isoquinolinone derivs. such as I (R = H, cyclopentyl, morpholino, etc.) designed by the comparison of the structure of cGMP and a previously reported 1-arylnaphthalene lignan, was disclosed. 4-Aryl-1-isoquinolinone derivs. such as the hydrochlorides of I (R = H, cyclopentyl, morpholino, etc.) were prepared and studied as potent and selective inhibitors of phosphodiesterase 5 (PDE5). I were designed by anal. of the structures of cGMP and a previously reported 1-arylnaphthalene lignan. Among these compds., the dihydrochloride of Me 2-(4-aminophenyl)-1,2-dihydro-1-oxo-7-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl)-3-isoquinoline carboxylate (II) exhibited potent PDE5 inhibitory activity (IC50 = 1.0 nM) with high isoenzyme selectivities (IC50 ratio: PDE1/PDE5 = 1300, PDE2/PDE5 > 10 000, PDE3/PDE5 > 10 000, PDE4/PDE5 = 4700, PDE6/PDE5 = 28). Compound II also showed the most potent

Updated Search

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relaxant effect on isolated rabbit corpus cavernosum (EC30 = 7.9 nM). Isoquinolinone compound III (T-1032), the sulfate salt of II, was selected for further biol. and pharmacol. evaluation of erectile dysfunction.

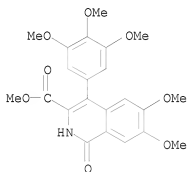
IT 212489-49-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of arylisoquinolinone derivs. as selective inhibitors of phosphodiesterase 5 and as potential agents for the treatment of erectile dysfunction)

RN 212489-49-1 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)



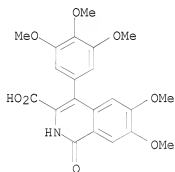
IT 212489-07-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of arylisoquinolinone derivs. as selective inhibitors of phosphodiesterase 5 and as potential agents for the treatment of erectile dysfunction)

RN 212489-07-1 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)



REFERENCE COUNT:

29

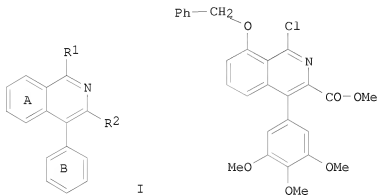
THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Updated Search

L6 ANSWER 13 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2000:712977 HCAPLUS  
 DOCUMENT NUMBER: 133:281699  
 TITLE: Preparation of isoquinoline derivatives as  
 phosphodiesterase V inhibitors  
 INVENTOR(S): Ukita, Shinzo; Yamada, Koichiro; Ohmori, Kenji;  
 Yoshikawa, Kohei  
 PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 49 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000281654	A	20001010	JP 1999-83022	19990326
PRIORITY APPLN. INFO.:			JP 1999-83022	19990326
OTHER SOURCE(S):	MARPAT	133:281699		

GI



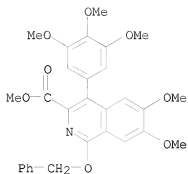
AB The title compds. I [ring A = benzene ring with substituents; ring B = (un)substituted benzene ring; R<sup>1</sup> = (un)substituted alkoxy, halo, etc.; R<sup>2</sup> = CO<sub>2</sub>R<sup>3</sup>, etc.; R<sup>3</sup> = H, etc.], useful as phosphodiesterase V inhibitors (no data) for the treatment of circulatory system diseases (no data), are prepared. For example, the title compound II was prepared.

IT 299167-15-0P 299167-17-2P 299167-19-4P  
 299167-21-8P 299167-23-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of isoquinoline derivs. as phosphodiesterase V inhibitors)

RN 299167-15-0 HCAPLUS

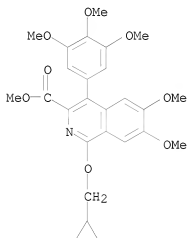
CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-(phenylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)

stn



RN 299167-17-2 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1-(cyclopropylmethoxy)-6,7-dimethoxy-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)

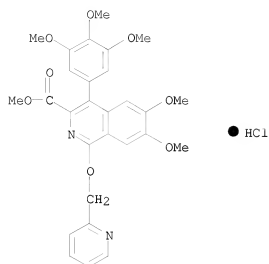


RN 299167-19-4 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-(2-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester, hydrochloride (1:1) (CA INDEX NAME)

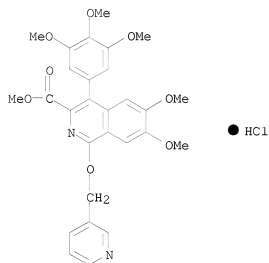
Updated Search

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RN 299167-21-8 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-(3-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester, hydrochloride (1:1) (CA INDEX NAME)

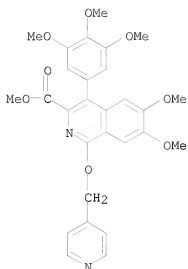


RN 299167-23-0 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 6,7-dimethoxy-1-(4-pyridinylmethoxy)-4-(3,4,5-trimethoxyphenyl)-, methyl ester, hydrochloride (1:1) (CA INDEX NAME)

Updated Search

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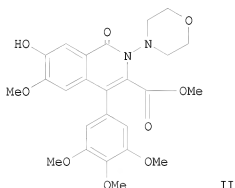
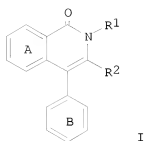


● HCl

L6 ANSWER 14 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2000:151451 HCAPLUS  
DOCUMENT NUMBER: 132:207769  
TITLE: Preparation of isoquinolinones as effective component  
in medicine  
INVENTOR(S): Ukita, Shinzo; Ohmori, Kanji; Ikeo, Tomihiro  
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 148 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000072675	A	20000307	JP 1998-240446	19980826
PRIORITY APPLN. INFO.:			JP 1998-240446	19980826
OTHER SOURCE(S):	MARPAT	132:207769		
GI				

stn

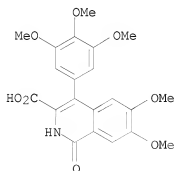


AB Title compds. [I; ring A and ring B equivalent or different, substituted or unsubstituted benzene ring; R1 = H, N(CH3)2, 4-H2NC6H4, 4-CH3OCOC6H4, alkyl, cycloalkyl, aryl, complex cyclic; R2 = COOH, COOCH3, COOCH2CH3, COOCH2C6H5, COO(CH2)3CH3] and pharmaceutical acceptable salts are prepared and tested as PDEV inhibitors. The title compound II was prepared

IT 212489-07-1P 212489-10-6P 212489-49-1P  
212500-07-7P 212500-10-2P  
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of isoquinolinones as effective component in medicine)

RN 212489-07-1 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

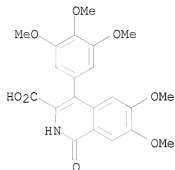


Updated Search

stn

RN 212489-10-6 HCAPLUS

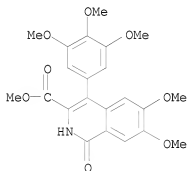
CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, sodium salt (1:1) (CA INDEX NAME)



● Na

RN 212489-49-1 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)



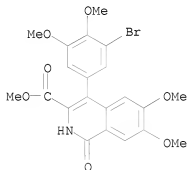
RN 212500-07-7 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo- (CA INDEX NAME)



COc1cc(OC)c(Br)cc1C1=CNC(=O)C2=CC(OC)=CC(OC)=C2C1=O

CN 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo-, methyl ester (CA INDEX NAME)

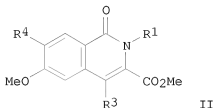
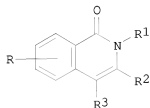


PATENT INFORMATION:

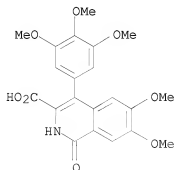
Updated Search

stn

US, UZ, VN, YU, ZW  
 RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI,  
 FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM,  
 GA, GN, ML, MR, NE, SN, TD, TG  
 IN 1998MA00345 A 20050304 IN 1998-MA345 19980220  
 AU 9862300 A 19980918 AU 1998-62300 19980223  
 JP 10298164 A 19981110 JP 1998-44139 19980226  
 PRIORITY APPLN. INFO.: JP 1997-44408 A 19970227  
 WO 1998-JP715 W 19980223  
 OTHER SOURCE(S): MARPAT 129:216521  
 GI



AB Title compds. [I; R = H or substituent(s); R1 = H, NH2, (cyclo)alkyl, heterocyclyl, aryl, etc.; R2 = (esterified) CO2H, CONH2, N-attached heterocyclcarbonyl, etc.; R3 = (un)substituted Ph] were prepared as PDE V inhibitors (no data). Thus, 5-benzyloxy-4-methoxy-2-(3,4,5-trimethoxybenzoyl)benzoic acid was cyclocondensed with CH2(CO2CMe3)2 and the hydrated product cyclocondensed with 4-(H2N)C6H4NHCOCMe3 to give, in 4 addnl. steps, title compound II [R1 = C6H4(NH2)-4, R3 = C6H2(OMe)3-3,4,5, R4 = 2-pyridylmethoxyl].  
 IT 212489-07-1P 212489-10-6P 212489-49-1P  
 212500-07-7P 212500-10-2P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of 1-isoquinolinone-3-carboxylates as PDE V inhibitors)  
 RN 212489-07-1 HCAPLUS  
 CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)- (CA INDEX NAME)

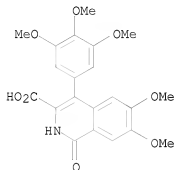


Updated Search

stn

RN 212489-10-6 HCAPLUS

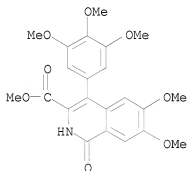
CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, sodium salt (1:1) (CA INDEX NAME)



● Na

RN 212489-49-1 HCAPLUS

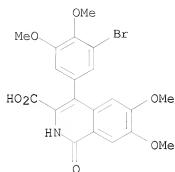
CN 3-Isoquinolinecarboxylic acid, 1,2-dihydro-6,7-dimethoxy-1-oxo-4-(3,4,5-trimethoxyphenyl)-, methyl ester (CA INDEX NAME)



RN 212500-07-7 HCAPLUS

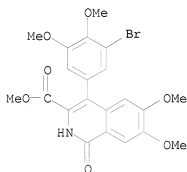
CN 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo- (CA INDEX NAME)

stn



RN 212500-10-2 HCAPLUS

CN 3-Isoquinolinecarboxylic acid, 4-(3-bromo-4,5-dimethoxyphenyl)-1,2-dihydro-6,7-dimethoxy-1-oxo-, methyl ester (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 16 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:211847 HCAPLUS

DOCUMENT NUMBER: 128:294669

ORIGINAL REFERENCE NO.: 128:58399a,58402a

TITLE: Synthesis of 7,12-dihydro-12-phenyl-5H-6,12-methanodibenz[c,f]azocines via N,N-dibenzylphenacylamines

AUTHOR(S): Coskun, Necdet; Buyukuysal, Levent

CORPORATE SOURCE: Dep. Chem., Uludag Univ., Bursa, 16059, Turk.

SOURCE: Heterocycles (1998), 48(1), 53-59

CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 128:294669

GI

Updated Search

stn

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB N,N-Dibenzylphenacylamines I (R1 = R2 = MeO, R3 = R4= R5 = R6 = H; R1 = R6 = H, R2 = R3 = R4 = R5 = MeO; R1R2 = OCH2O, R3 = R6 = H, R4 = R5 = MeO; etc.) were prepared in high yields by a one-pot reaction and cyclized at room temperature to give 7,12-dihydro-12-phenyl-5H-6,12-methanodibenz[c,f]azocines II in high yields. 95% H2SO4 or 70% HClO4 was used as cyclization catalysts. The double-cyclization proceeds smoothly in the cases where electron-donating groups are present in both benzene rings. N-2,3-dimethoxybenzyl-N-benzylphenacylamine gave the corresponding N-benzyl-1,2-dihydro-4-phenylisoquinoline on treatment with 95% H2SO4 while N-3,4-dimethoxybenzyl-N-benzylphenacylamine at the same reaction conditions and reaction time cyclized to the corresponding dibenzazocine. However, N-3,4-dimethoxybenzyl-N-benzylphenacylamine gave the corresponding dihydroisoquinoline which disproportionates to give N-benzyl-1,2,3,4-tetrahydro-4-phenylisoquinoline and N-benzyl-4-phenylisoquinolinium when treated with 70% perchloric acid at room temperature

IT 206126-10-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of phenylmethanodibenzazocines by cyclization of dibenzylphenacylamines)

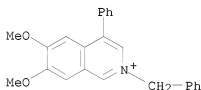
RN 206126-10-5 HCAPLUS

CN Isoquinolinium, 6,7-dimethoxy-4-phenyl-2-(phenylmethyl)-, perchlorate (1:1) (CA INDEX NAME)

CM 1

CRN 206126-09-2

CMF C24 H22 N O2



CM 2

CRN 14797-73-0

CMF Cl O4



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Updated Search

stn

L6 ANSWER 17 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:224821 HCAPLUS

DOCUMENT NUMBER: 104:224821

ORIGINAL REFERENCE NO.: 104:35659a,35662a

TITLE: The synthesis of a 4-phenylisoquinoline from a 3-phenylisoquinoline by utilization of a nitrogen analog of the pinacol rearrangement

AUTHOR(S): Cushman, Mark; Mohan, Prem

CORPORATE SOURCE: Sch. Pharm. Pharm. Sci., Purdue Univ., West Lafayette, IN, 47907, USA

SOURCE: Tetrahedron Letters (1985), 26(38), 4563-6

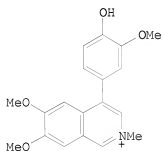
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

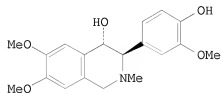
LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:224821

GI



I



II

AB The nitrogen analog of the pinacol rearrangement was used for the preparation of a 4-phenylisoquinoline I from the intermediate amino alc. II.

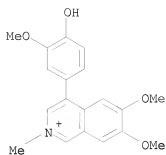
IT 102349-19-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 102349-19-9 HCAPLUS

CN Isoquinolinium, 4-(4-hydroxy-3-methoxyphenyl)-6,7-dimethoxy-2-methyl-, chloride (1:1) (CA INDEX NAME)

stn



L6 ANSWER 18 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:527463 HCAPLUS

DOCUMENT NUMBER: 97:127463

ORIGINAL REFERENCE NO.: 97:21153a,21156a

TITLE: A reinvestigation of the Pictet-Gams isoquinoline synthesis. Part 2. Formation of rearranged isoquinolines: the A2-oxazoline-isoquinoline transformation

AUTHOR(S): Ardabilchi, Nasser; Fitton, Alan O.; Haidi, A. Hamid b. A.; Thompson, J. Robin

CORPORATE SOURCE: Dep. Chem. Appl. Chem., Univ. Salford, Salford, M5 4WT, UK

SOURCE: Journal of Chemical Research, Synopses (1982), (6), 156-7

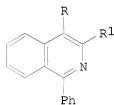
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

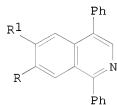
LANGUAGE: English

OTHER SOURCE(S): CASREACT 97:127463

GI



I



II

AB Cyclization of 2-substituted 2-acylamino-1-arylalkan-1-ols with P205 in refluxing decalin gave rearranged, i. e., 4-substituted, isoquinolines in addition to the expected 3-substituted isomers. E.g., erythro-PhCH(OH)CH(CHMe<sub>2</sub>)NHBz cyclized to give 37% of a 31:69 mixture of isoquinolines I (R = H, R<sub>1</sub> = CHMe<sub>2</sub>; R = CHMe<sub>2</sub>, R<sub>1</sub> = H). With erythro-PhCH(OH)CHRNHBz (R = C<sub>6</sub>H<sub>4</sub>OMe-3, -4), the 4-substituted isoquinolines II (R = H, R<sub>1</sub> = OMe; R = OMe, R<sub>1</sub> = H), resp., were obtained

Updated Search

stn

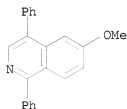
exclusively in 76 and 88% yields. The reaction involves 5-phenyl- $\Delta^2$ -oxazoline intermediates; the formation of the rearranged isoquinolines from the intermediates is discussed.

IT 82894-69-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 82894-69-7 HCAPLUS

CN Isoquinoline, 6-methoxy-1,4-diphenyl- (CA INDEX NAME)



L6 ANSWER 19 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:125225 HCAPLUS

DOCUMENT NUMBER: 82:125225

ORIGINAL REFERENCE NO.: 82:20003a,20006a

TITLE: Formation of some isochromene derivatives during the reaction of veratryl ketones and veratric acid with benzoin

AUTHOR(S): Kuznetsov, E. V.; Pruchkin, D. V.; Bicherov, A. V.; Dorofeenko, G. N.

CORPORATE SOURCE: Rostov. Gos. Univ., Rostov-on-Don, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (1974), (11), 1575

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI For diagram(s), see printed CA Issue.

AB Benzopyrylium perchlorates (I; R = Me, Ph, p-MeOC<sub>6</sub>H<sub>4</sub>) were obtained in 40-60% yields by heating 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>COR with PhCH(OH)COPh in the presence of polyphosphoric acid 1 hr at 120-30°. Treatment of I with NH<sub>4</sub>OAc gave isoquinolines (II). Treatment of veratric acid with benzoin similarly gave 12% isocoumarin (III) which could be transformed into I (R = Me) by MeMgI.

IT 27922-95-8P 55542-77-3P 55542-78-4P

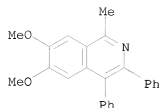
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 27922-95-8 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)

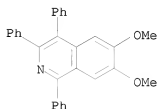


stn



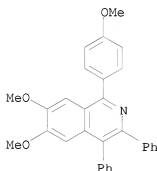
RN 55542-77-3 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1,3,4-triphenyl- (CA INDEX NAME)



RN 55542-78-4 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-(4-methoxyphenyl)-3,4-diphenyl- (CA INDEX NAME)



L6 ANSWER 20 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1970:132239 HCAPLUS

DOCUMENT NUMBER: 72:132239

ORIGINAL REFERENCE NO.: 72:23667a,23670a

TITLE: Use of polyphosphoric acid in the synthesis of  
o,o-diaryl-substituted acetophenones;  
3,4-diaryl-substituted 2-benzopyrylium salts and  
isoquinolines based on them

AUTHOR(S): Kuznetsov, E. V.; Dorofeenko, G. N.

CORPORATE SOURCE: Rostov.-na-Donu Gos. Univ., Rostov-on-Don, USSR

SOURCE: Zhurnal Organicheskoi Khimii (1970), 6(3), 578-81  
CODEN: ZORKAE; ISSN: 0514-7492

Updated Search

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DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

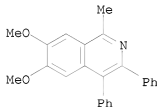
AB Condensation of veratrole with BZCH(OH)Ph, PhCH(OH)CO<sub>2</sub>H, or BZCHO in polyphosphoric acid gave 62-8% 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>-CHRCOR<sub>1</sub> (I) (R, R<sub>1</sub> given): Ph, Ph; Ph, 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>; 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, Ph; resp. Heating I (R = R<sub>1</sub> = Ph) with Ac<sub>2</sub>O and HClO<sub>4</sub> gave 6,7-dimethoxy-3,4-diphenyl-1-methyl-2-benzopyrylium perchlorate. Similarly, 6,7-dimethoxy-1,3,4-triphenyl-2-benzopyrylium and 6,7-dimethoxy-1-benzyl-3,4-diphenyl-2-benzopyrylium perchlorates were prepared 6,7-Dimethoxy-3,4-diphenyl-1-methylisoquinoline, and 1-benzyl-6,7-dimethoxy-3,4-diphenylisoquinoline were prepared from NH<sub>3</sub> and the resp. perchlorate.

IT 27922-95-8P 27922-96-9P 27922-97-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

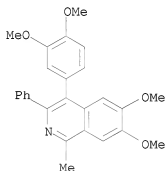
RN 27922-95-8 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-methyl-3,4-diphenyl- (CA INDEX NAME)



RN 27922-96-9 HCAPLUS

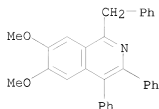
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-3-phenyl-  
(CA INDEX NAME)



RN 27922-97-0 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-3,4-diphenyl-1-(phenylmethyl)- (CA INDEX  
NAME)

stn



L6 ANSWER 21 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:50634 HCAPLUS

DOCUMENT NUMBER: 52:50634

ORIGINAL REFERENCE NO.: 52:9128d-h

TITLE: Synthesis of derivatives of

4-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline

AUTHOR(S): Quelet, Raymond; Mansouri, Mehdi; Pineau, Robert

CORPORATE SOURCE: Fac. Sci., Paris

SOURCE: Compt. rend. (1957), 245, 537-9

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:50634

AB An earlier note (C.A. 50, 8535e) described the condensation of veratrole with aminodiethylacetal to give 1,1-bis-(3,4-dimethoxyphenyl)-2-aminoethane (I) (80% yield) in AcOH in the presence of H<sub>2</sub>SO<sub>4</sub>. The N-Ac, N-Pr, and N-Bu derivs. (II) of I were obtained when the corresponding N-acylaminoacetals were used in the condensation. Compound I and its N-acyl derivs. were transformed into isoquinolines in order to compare the physiological properties of these products with those of papaverine. Using the method of Pictet and Spengler (C.A. 5, 3423) 5 g. I, 10 cc. MeOH, 5 cc. 40% formalin, and 10 cc. concentrated HCl was mixed and refluxed 2 hrs. giving 70% 6,7-dimethoxy-4-(3,4-dimethoxyphenyl)-1,2,3,4-tetrahydroisoquinoline (III), m. 147° (MeOH); HCl salt, m. 240°; picrate, m. 233°. An attempt at Pd-catalyzed dehydrogenation of III was unsuccessful. II refluxed with POC13 in toluene (method of Pictet and Finkelstein, C.A. 3, 2435; Ber. 42, 1979 (1909), and Decker, and Kropp, C.A. 3, 2455) gave 3,4-dihydro-6,7-dimethoxy-4-(3,4-dimethoxyphenyl)-1-alkyl (or aryl) isoquinolines (IV), yield 60-75%. The following IV were reported (1-substituent, m.p. of base, HCl salt, and picrate given): Me, 70°, 191-2°, 220-1°; Et, 129°, -, 190-1°; Ph, 129-30°, 163-4°, 167-8°. IV were dehydrogenated in 80% yield to the corresponding isoquinolines (V) by Pd in boiling PhMe. The following V were reported (1-substituent, m.p. of base, HCl salt, and picrates given): Me, 207-8°, 211-12°, 240°; Et, 176°, -, 222-3°; Ph, 105-7°, -, 224°.

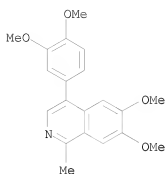
IT 102012-78-2 102948-36-7

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 102012-78-2 HCAPLUS

CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-, hydrochloride (1:1) (CA INDEX NAME)

stn



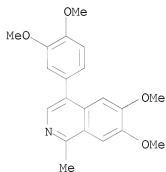
● HCl

RN 102948-36-7 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-, compd. with  
2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 102012-79-3

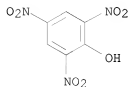
CMF C20 H21 N O4



CM 2

CRN 88-89-1

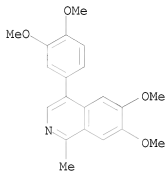
CMF C6 H3 N3 O7



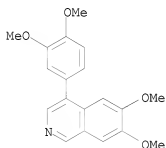
Updated Search

stn

IT 102012-79-3, Isoquinoline,  
4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-  
(and derivs.)  
RN 102012-79-3 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX  
NAME)



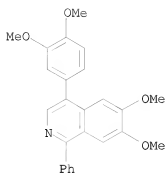
IT 109614-11-1, Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-  
(derivs.)  
RN 109614-11-1 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)



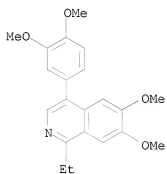
IT 102891-93-0P, Isoquinoline,  
4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-phenyl- 111719-66-5P,  
Isoquinoline, 4-(3,4-dimethoxyphenyl)-1-ethyl-6,7-dimethoxy-  
114839-77-9P, Isoquinoline,  
4-(3,4-dimethoxyphenyl)-1-ethyl-6,7-dimethoxy-, picrate  
115485-51-3P, Isoquinoline,  
4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-phenyl-, picrate  
RL: PREP (Preparation)  
(preparation of)  
RN 102891-93-0 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-phenyl- (CA INDEX  
NAME)

Updated Search

stn



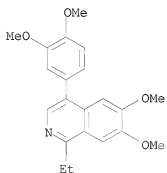
RN 111719-66-5 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-1-ethyl-6,7-dimethoxy- (CA INDEX NAME)



RN 114839-77-9 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-1-ethyl-6,7-dimethoxy-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 111719-66-5  
CMF C21 H23 N O4



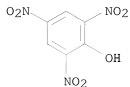
Updated Search

stn

CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



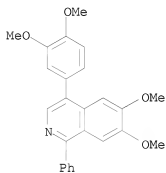
RN 115485-51-3 HCAPLUS

CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-phenyl-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 102891-93-0

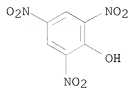
CMF C25 H23 N 04



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L6 ANSWER 22 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

Updated Search

stn

ACCESSION NUMBER: 1958:50633 HCAPLUS  
DOCUMENT NUMBER: 52:50633  
ORIGINAL REFERENCE NO.: 52:9128b-d  
TITLE: Reaction of phenyl- and p-tolyl lithium with  
1-arylisquinolines  
AUTHOR(S): Gilman, Henry; Soddy, Theodore  
CORPORATE SOURCE: Iowa State Coll., Ames  
SOURCE: Journal of Organic Chemistry (1957), 22, 1716-17  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

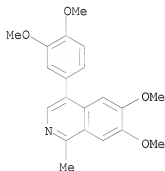
AB The addition of aryllithium reagents to 1-arylisquinolines was studied. 1-p-Tolyl- (I) and 1-phenylisquinoline (II) treated with PhLi (III) and p-MeC<sub>6</sub>H<sub>4</sub>Li (IV), resp., gave in each case 1-phenyl-p-(1-tolyl)-1,2-dihydroisquinoline (V). This fact was demonstrated by mixed decomposition point and identical infrared spectra. Both of the spectra contained a 1,4-disubstituted Ph band at 12.3  $\mu$ , a Ph ring band at 6.15  $\mu$ , and an NH band at 3.1  $\mu$ . II (16 g.) in 200 ml anhydrous Et<sub>2</sub>O was treated dropwise with 0.08 mole IV in 90 ml. Et<sub>2</sub>O; after the addition of 2, 5, and 8 ml. IV solution the reaction became red, brown, and finally dark green in color; the green color was present throughout the remainder of the addition. On completion of the addition the mixture refluxed

45 min., hydrolyzed with saturated NH<sub>4</sub>Cl, and the Et<sub>2</sub>O extract dried, the Et<sub>2</sub>O removed, and the residue dissolved in alc., treated with C, filtered, and evaporated gave 0.5 g. V, decompose 176-8°. I (19 g.) in 200 ml. Et<sub>2</sub>O treated with 0.09 mole III in 100 ml. Et<sub>2</sub>O and the mixture worked up as in the preceding method gave 0.5 g. V.

IT 102012-78-2 102948-36-7  
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 102012-78-2 HCAPLUS

CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

RN 102948-36-7 HCAPLUS

CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

Updated Search

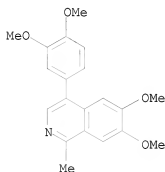


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CM 1

CRN 102012-79-3

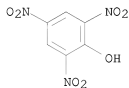
CMF C20 H21 N O4



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L6 ANSWER 23 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:40607 HCAPLUS

DOCUMENT NUMBER: 52:40607

ORIGINAL REFERENCE NO.: 52:7320a-i,7321a

TITLE: Cyclic nitrones. II. Polymers of 2,3,4,5-tetrahydropyridine N-oxide and related compounds

AUTHOR(S): Thesing, Jan; Mayer, Hans

CORPORATE SOURCE: Tech. Hochschule, Darmstadt, Germany

SOURCE: Justus Liebigs Annalen der Chemie (1957), 609, 46-57

CODEN: JLACBF; ISSN: 0075-4617

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 52:40607

AB cf. C.A. 51, 10516a. N-Hydroxypiperidine (Ia) (0.04 mole) with 0.2 mole KOH in 50 cc. H2O at 20-5° was treated dropwise with 0.08 mole K3Fe(CN)6 in 80 cc. H2O, diluted with H2O and kept 2 hrs. at 20° in the dark, cooled to 0° saturated with K2CO3, and extracted with CHCl3 giving 97% (C5H9ON)3 (I) (mol. weight in C6H6 268-318), exploding on

Updated Search

attempted distillation in vacuo, pH 8-9 in H<sub>2</sub>O. After standing 3 weeks, I gave an orange mass, which in aqueous Me<sub>2</sub>CO cooled to -15° yielded 41% (C<sub>5</sub>H<sub>9</sub>ON)<sub>2</sub> (II), m. 126-7° (described previously, loc. cit.), and unidentified high polymers. I (0.85 g.) within 2 hrs. after preparation was hydrogenated in 75 cc. N HCl with PtO<sub>2</sub> at 20°/760 mm. giving 98.5% (crude yield) Ia.HCl, m. 142-3°. II (0.3 g.) in 20 cc. 2N HCl was added promptly to 40 cc. 20% NaOH at 20°, cooled to 0°, saturated with K<sub>2</sub>CO<sub>3</sub>, and extracted with CHCl<sub>3</sub> giving I quantitatively. When

II

in HCl was kept 12 hrs. prior to treatment with NaOH, the mol. weight of the resulting product rose from 297 to 402. To 26.7 g. PhMgBr in 70 cc. absolute Et<sub>2</sub>O was added dropwise freshly prepared I in 100 cc. Et<sub>2</sub>O and the mixture refluxed 4 hrs. giving a brown oil crystallizing gradually at 20°, which was decomposed with alkaline aqueous NH<sub>4</sub>Cl and extracted with Et<sub>2</sub>O yielding

2-Ph derivative

(III) of Ia, m. 111-12° (petr. ether) (described previously, loc. cit.). III (6.2 g.) in 160 cc. Me<sub>2</sub>CO and 16 cc. H<sub>2</sub>O was treated within 1-2 min. with 15.2 g. yellow HgO, shaken 1.5 hrs., kept 16 hrs., filtered, and washed with Me<sub>2</sub>CO. The evaporated filtrate gave 6.13 g. oil which after 6 days at 0° triturated with little AcOEt gave 1.76 g. colorless dimer (IV) of the 2,3,4,5-tetrahydro-2-phenylpyridine N-oxide, C<sub>22</sub>H<sub>26</sub>O<sub>2</sub>N<sub>2</sub>, m. 200-1° (decomposition) (iso-Am<sub>2</sub>O); the m.p. varies with rate of heating. In weakly alkaline solution IV gradually gave a pink color with triphenyltetrazolium chloride (V). IV (0.4 g.) in hot iso-Am<sub>2</sub>O with 0.8 g. PhMgBr in 10 cc. Et<sub>2</sub>O was refluxed and stirred at 110-20°, cooled, decomposed with NH<sub>4</sub>Cl in dilute NH<sub>4</sub>OH, and extracted with Et<sub>2</sub>O giving

0.56

g. oil, which triturated with MeOH gave 0.21 g. 6-Ph derivative (VI) of III, m. 165-6° (EtOH), giving an immediate red color with V. VI (0.25 g.) in 25 cc. warm H<sub>2</sub>O and 6 cc. HCl heated 3 hrs. at 100° with Zn dust, cooled, and made alkaline with concentrated NaOH gave 0.22 g. crude iso-2,6-diphenylpiperidine, identified as the HCl salt, m. 224-5°; HBr salt, m. 258-9°, and HI salt, m. 256-7° (cf. Gilman and Edward, C.A. 48, 3974f), identical with those prepared from 2,6-diphenylpyridine reduced with EtOH and Na. To 16.8 g. 1,2,3,4-tetrahydroisoquinoline (VII) was added dropwise 12.8 g. CH<sub>2</sub>:CHCO<sub>2</sub>Et and the mixture heated 1 hr. at about 90-100° giving 24.25 g. N-carbethoxyethyl-1,2,3,4-tetrahydroisoquinoline (VIII), b<sub>15</sub> 188-9°. To 12 g. VIII in 100 cc. absolute Et<sub>2</sub>O at 0-5° was added 180 cc. Et<sub>2</sub>O containing o-HO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>CO<sub>3</sub>H [Organic Syntheses, Collective Volume III, 619(1955)] giving a viscous oil from which the Et<sub>2</sub>O solution (IX) was decanted. The oil in 100 cc. 2N NaOH saturated with K<sub>2</sub>CO<sub>3</sub>

was

heated 1 hr. at 80-90°, diluted with 100 cc. H<sub>2</sub>O, and extracted with Et<sub>2</sub>O (including extract IX) giving 37-45% crude 2-hydroxy-1,2,3,4-tetrahydroisoquinoline (X), purified through its HCl salt, m. 153-4° (Me<sub>2</sub>CO); this with aqueous NaOH gave X, m. 80-1° (cyclohexane), giving an immediate red color with V [picrate of X, m. 143-4° (H<sub>2</sub>O)]. Crude X decomposed rapidly in a desiccator; pure X proved quite stable. X, prepared from VII in aqueous Me<sub>2</sub>CO with H<sub>2</sub>O<sub>2</sub>, was obtained in only 2% yield [cf. Maass and Wolfenstein, Ber. 30, 2189(1897) and 31, 2687(1898) who termed X "o-aminomethylphenylacetaldehyde" (m. 76-7°)]. X (0.48 g.) in 15 cc. Me<sub>2</sub>CO and 1.5 cc. H<sub>2</sub>O was shaken 1.5 hrs. with 1.4 g. HgO; the evaporated filtrate gave the crude nitron, 3,4-dihydroisoquinoline N-oxide (XI), purified through the picrate, m. 142.5-3.5° (MeOH), 0.84 g. of which was warmed at

stn

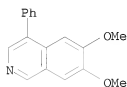
50° with 18% HCl, extracted with PhNO<sub>2</sub> and Et<sub>2</sub>O, and the aqueous phase poured into 40 cc. 2N NaOH at 0° over a layer of CHCl<sub>3</sub>, saturated with K<sub>2</sub>CO<sub>3</sub>, and well shaken. The CHCl<sub>3</sub> extract gave 0.3 g. hygroscopic XI, m. 56-7° (after evaporation, keeping 14 days at 0°, triturating with absolute Et<sub>2</sub>O, and drying over P<sub>2</sub>O<sub>5</sub>). XI gave no color with V. The marked differences in the HgO dehydrogenations of III and X are discussed fully and explained on the basis of configurational analyses. Ultraviolet spectra of XI and of benzaldehyde N-methylnitron and the infrared spectrum of IV are given and discussed. 27 references.

IT 108973-36-0 112685-68-4

(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 108973-36-0 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-4-phenyl- (CA INDEX NAME)



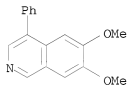
RN 112685-68-4 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-4-phenyl-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 108973-36-0

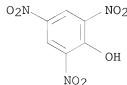
CMF C17 H15 N O2



CM 2

CRN 88-89-1

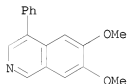
CMF C6 H3 N3 O7



Updated Search

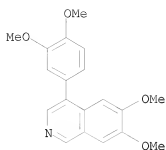
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L6 ANSWER 24 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1958:40606 HCAPLUS  
DOCUMENT NUMBER: 52:40606  
ORIGINAL REFERENCE NO.: 52:7319h-i,7320a  
TITLE: Syntheses of isoquinoline derivatives of  
pharmacological interest  
AUTHOR(S): Deshpande, V. N.; Nargund, K. S.  
CORPORATE SOURCE: Karnatak Univ., Dharwar, India  
SOURCE: Journal of the Karnatak University (1956), 1, 15-18  
CODEN: JKAUAR; ISSN: 0453-3348  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB The  $\beta,\beta$ -diarylsubstituted ethylamine (0.005 mole) was treated  
with 40% formalin (slight excess over 0.008 mole). The intermediate  
Schiff bases were obtained as pastes and were cyclized by the action of  
24% HCl. Isoquinoline bases thus formed were characterized by the  
formation of picrates. The bases (0.250 g.) were dehydrogenated by 10%  
Pd-C by heating the mixture at 210-15° for 15 min. and the resulting  
isoquinoline derivs. were isolated as the picrate. Below are given  
comps. and m.ps. of the tetrahydroisoquinoline base, its picrate, and the  
picrate of the isoquinoline base: 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-  
1,2,3,4-tetrahydroisoquinoline, 106°, 195°, 269°;  
4-(4-methoxyphenyl)-7-methoxy-1,2,3,4-tetrahydroisoquinoline, 92°,  
240°, 168°; 4-phenyl-6,7-dimethoxy-1,2,3,4-  
tetrahydroisoquinoline, 173°, 219°, 236°;  
4-(4-methoxyphenyl)-1,2,3,4-tetrahydroisoquinoline, 76°,  
163°, 244°; 4-(2,4-dimethoxyphenyl)-1,2,3,4-  
tetrahydroisoquinoline, 182°, 230°, 204°.  
IT 108973-36-0P, Isoquinoline, 6,7-dimethoxy-4-phenyl-  
109614-11-1P, Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-  
112685-68-4P, Isoquinoline, 6,7-dimethoxy-4-phenyl-, picrate  
113751-11-4P, Isoquinoline,  
4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-, picrate  
RL: PREP (Preparation)  
(preparation of)  
RN 108973-36-0 HCAPLUS  
CN Isoquinoline, 6,7-dimethoxy-4-phenyl- (CA INDEX NAME)



RN 109614-11-1 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy- (CA INDEX NAME)

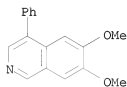
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RN 112685-68-4 HCAPLUS  
CN Isoquinoline, 6,7-dimethoxy-4-phenyl-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

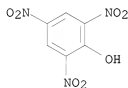
CM 1

CRN 108973-36-0  
CMF C17 H15 N O2



CM 2

CRN 88-89-1  
CMF C6 H3 N3 O7



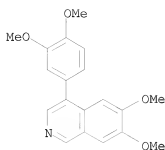
RN 113751-11-4 HCAPLUS  
CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-, compd. with 2,4,6-trinitrophenol (1:1) (CA INDEX NAME)

CM 1

CRN 109614-11-1  
CMF C19 H19 N O4

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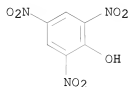
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CM 2

CRN 88-89-1

CMF C6 H3 N3 O7



L6 ANSWER 25 OF 25 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1955:53526 HCAPLUS

DOCUMENT NUMBER: 49:53526

ORIGINAL REFERENCE NO.: 49:10280f-i,10281a-i,10282a-i,10283a-d

TITLE: Hypotensive methoxyisoquinolines

AUTHOR(S): Walker, Gordon N.

CORPORATE SOURCE: Natl. Heart Inst., Bethesda, MD

SOURCE: Journal of the American Chemical Society (1954), 76, 3999-4003

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Dehydronorcoralydine iodide (I) was synthesized. The HCl salts of 3-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline (II), 1-methyl-4-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline (III), 1-methyl-4-phenyl-6,7-dimethoxyisoquinoline (IV), 1-methyl-6,7-dimethoxyisoquinoline (V), and 5-methyl-2,3,10,11-tetramethoxybenzo[a]-phenanthridine (VI) were prepared by the POCl<sub>3</sub> cyclization of the appropriate amides, dehydrogenation, and treatment with HCl. These compds. elicited a lowering of the blood pressure in normal dogs. N-(3,4-Dimethoxyphenylacetyl)homoveratrylamine (40 g.) refluxed 3 h. with 100 cc. POCl<sub>3</sub> in 800 cc. PhMe, the mixture treated with excess alc. KOH, and diluted with H<sub>2</sub>O, and the product triturated with MeOH gave 30 g. (76%) 1-(3,4-dimethoxybenzoyl)-6,7-dimethoxy-3,4-dihydroisoquinoline (3,4-dihydropapaveraldine) (VII), m. 185-9° (recrystd. from EtOAc, colorless crystals, m. 190-2°) (all m.ps. are corrected), λ<sub>maximum</sub> 6.03, 6.25-6.40 μ. VII (30 g.) in 250 cc. glacial AcOH hydrogenated at

80° and 40 lb. pressure over 4.5 g. 10% Pd-C 5 h. (the catalyst was renewed twice during this period), the mixture filtered, the AcOH evaporated, the residual viscous oil dissolved in Et<sub>2</sub>O-MeOH, the solution saturated with cooling with HCl, and the resulting crystals triturated with absolute EtOH and dried in air yielded 22.2 g. (67%) 1,2,3,4-tetrahydropapaverine (VIII) HCl salt, colorless crystals, m. 195-206° [recrystd. from MeOH, m. 212-14° (decomposition)]. VIII.HCl (21 g.) in 300 cc. H<sub>2</sub>O and 7 cc. concentrated HCl treated with 20 cc. CH<sub>2</sub>O, the mixture heated 1 h. on the steam bath, the solution diluted with 400 cc. H<sub>2</sub>O, cooled, treated with excess KOH, refrigerated overnight, and filtered, the filter residue triturated with 150 cc. warm MeOH, the MeOH extract evaporated, and the residue recrystd. from

75

cc. MeOH yielded 7.3 g. (37%) crude product, m. 151-6°, which recrystd. from MeOH gave pure norcoralydine (IX) hemihydrate, colorless crystals, m. 159-61°; the MeOH-insol. crystals (8.0 g., 41%), m. 174-97° (decomposition), recrystd. from EtOAc gave 5.6 g. unidentified product, slightly greenish crystals (X), m. 202-5° [recrystd. m. 203-6° (partial decomposition)],  $\lambda_{\text{maximum}}$  2.82-2.85, 7.2, 9.1  $\mu$ . IX and X showed very similar IR spectra. IX (2.0 g.) treated in 300 cc. absolute EtOH with 5.5 g. iodine, the mixture refluxed 4 h., cooled, and filtered, the filter residue triturated several times with warm EtOAc, the resulting deep red complex, decomposing 223-6°, which could not be recrystd. because of decomposition, warmed with aqueous NaHSO<sub>3</sub>, and the

resulting

yellow crystals washed with dilute HCl and H<sub>2</sub>O, dried in air, and recrystd. from MeOH gave 1.4 g. I, yellow crystals, m. 222.5-26° (decomposition) (varied with rate of heating), which appeared to be solvated. X treated with iodine in the same manner, and the resulting red complex, decomposing 222.5-26°, treated with aqueous NaHSO<sub>3</sub> yielded I, m. 252-4° (decomposition) (from MeOH); mixed m.p. with I from IX, 252-5° (decomposition). I caused with 1.0 mg./kg. dog a slight and with 31 mg./kg. a marked fall of the blood pressure, with 15 mg./kg. a partial epinephrine block, with 7 mg. a partial TMA block; the fatal dose was 63 mg./kg.; it caused also tachycardia. Homoveratroyl chloride treated with veratrole in the presence of AlCl<sub>3</sub> in CS<sub>2</sub>, and the mixture distilled gave 31% 3,3',4,4'-tetramethoxydeoxybenzoin (XI), colorless crystals, m. 104-6° (from MeOH), b.p. 240-70°; 2,4-dinitrophenylhydrazones, red-orange crystals, m. 197-9° (from EtOAc). XI treated with NH<sub>2</sub>OH.HCl in pyridine gave the oxime of XI, colorless crystals, m. 129-31°; the hydrogenation of the oxime in EtOH and EtOAc over Pd-C gave products which were not identical with  $\alpha,\beta$ -di(3,4-dimethoxyphenyl)ethylamine (XII). 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CHO (81 g.), 101 g. 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>CO<sub>2</sub>H, 50.5 g. KOAc, and 230 cc. Ac<sub>2</sub>O refluxed 2 h., the solution diluted with 100 cc. MeOH and 2000 cc. H<sub>2</sub>O, and the precipitate washed with H<sub>2</sub>O, pressed dry, and triturated with Et<sub>2</sub>O gave 98 g. (58%) 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>[3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>]CCO<sub>2</sub>H (XIII), colorless crystals, m. 204-13° (recrystd. from EtOAc, m. 216-17°). XIII in glacial AcOH hydrogenated at 70° over 5% Pd-C, the mixture filtered, the filtrate evaporated, and the crude product (100%) recrystd. from MeOH gave  $\alpha,\beta$ -di(3,4-dimethoxyphenyl)propionic acid (XIV), colorless crystals, m. 143-5°. XIV (83 g.) esterified with absolute EtOH in the presence of 5% concentrated H<sub>2</sub>SO<sub>4</sub> yielded 73 g. (81%) crude Et ester (XV) of XIV, oil. BzCl (81.5 g.), 69.5 g. veratrole, and 89 g. AlCl<sub>3</sub> in 300 cc. CS<sub>2</sub> condensed in the usual manner, the resulting complex decomposed with ice and H<sub>2</sub>O, and the neutral product recrystd. from MeOH in 2 crops yielded 83 g. (68%) 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>Bz (XVI), m. 98-100°;

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2,4-dinitrophenylhydrazone, red crystals, m. 256-7° (from EtOAc).

XVI (41.3 g.), 36 g. BrCH<sub>2</sub>CO<sub>2</sub>Et, 50 g. activated Zn (30 mesh), and 500 cc. dry C<sub>6</sub>H<sub>6</sub> refluxed 4 h., the mixture decomposed with dilute AcOH, the neutral product isolated in the usual manner and hydrogenated in glacial AcOH at 80° 1 h. over 10% Pd-C at 40 lb. pressure, the mixture filtered, and the filtrate evaporated gave 100% crude 3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CHPhCH<sub>2</sub>CO<sub>2</sub>Et, orange oil, suitable for further conversions. XI (23 g.), 200 cc. HCONH<sub>2</sub>, 100 cc. 90% HCO<sub>2</sub>H, and 50 g. HCO<sub>2</sub>NH<sub>4</sub> distilled until the reflux temperature reached 165°, the mixture refluxed 9 h., cooled, and diluted with 3000 cc. H<sub>2</sub>O, and the crystalline precipitate washed with H<sub>2</sub>O and recrystd. from MeOH yielded 14 g.

(56%) N-CHO derivative (XVIII) of XII, m. 138-41° (recrystd. from

MeOH, m. 141-3°), λ<sub>maximum</sub> 2.95, 5.94 μ. XIV refluxed 3 h.

with 2 parts by weight anhydrous N<sub>2</sub>H<sub>4</sub>, the solution cooled and poured into 20

vols.

ice water, and the crystalline precipitate washed with several portions H<sub>2</sub>O and dried

in vacuo at room temperature yielded the hydrazide of XIV, colorless crystals, m. 140-2° (from MeOH). [3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CHCH<sub>2</sub>CONHNH<sub>2</sub>, colorless crystals, m. 240-2°, was obtained similarly from

[3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>]2CHCH<sub>2</sub>CO<sub>2</sub>Et; in the same manner was prepared

3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CHPhCH<sub>2</sub>CONHNH<sub>2</sub>, colorless crystals, m. 113-15° (from

MeOH), from XVII; and 1-(3,4-dimethoxyphenyl)-2-carboxy-6,7-

dimethoxytetralin hydrazide (XIX), colorless, hygroscopic crystals, m.

180-1° (from MeOH, dried in vacuo at 100°), from the Et

ester of the corresponding acid. Each of the hydrazides showed IR

absorption bands at 2.94 and 5.98 μ. The acid hydrazide (0.1 mol) in

300 cc. glacial AcOH, 200 cc. concentrated HCl, and 200 cc. H<sub>2</sub>O treated with

600

cc. Et<sub>2</sub>O to form a 2nd phase, the mixture treated with cooling and stirring with 20 g. NaNO<sub>2</sub> gradually during 0.5 h., diluted with 1 l. ice water, and shaken, the organic layer washed 4 times with H<sub>2</sub>O, with 3% aqueous NaOH until alkaline, and then with dilute AcOH, aqueous NaHCO<sub>3</sub>, and H<sub>2</sub>O, dried with MgSO<sub>4</sub>, treated immediately with 75 cc. glacial AcOH and 50 cc. Ac<sub>2</sub>O, and cautiously distilled to remove the Et<sub>2</sub>O, the residual liquid refluxed 2 h., the excess reagent evaporated, the residue treated with an equal volume Et<sub>2</sub>O

containing

a little Et<sub>2</sub>O, and the product recrystd. gave the rearrangement product.

In this manner were prepared the N-Ac derivative (XX) of XII, m. 148-65°

(recrystd. from EtOAc, colorless crystals, m. 160-3°), in 61% from

XIII, λ<sub>maximum</sub> 2.94, 6.00 μ [XX gave hydrolyzed 4 h. with KOH in

aqueous (HOCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>O XII, colorless crystals, m. 106-10° (from EtOAc)];

[3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>]2CHCH<sub>2</sub>NHAc (XXI), colorless crystals, m. 129-31°

(from MeOH), in 52% yield from XI, λ<sub>maximum</sub> 2.94, 6.01 μ;

3,4-(MeO)<sub>2</sub>C<sub>6</sub>H<sub>3</sub>CHPhCH<sub>2</sub>NAc (XXII), colorless crystals, m. 154-6°

(from MeOH), in 46% yield from XVI; and

1-(3,4-dimethoxyphenyl)-2-acetylamino-6,7-dimethoxytetralin (XXIII), m.

217-20° (recrystd. from MeOH, pale green crystals, m.

222-3.5°), in 73% yield from XIX, λ<sub>maximum</sub> 2.90, 6.00 μ.

The appropriate amide and dry PhMe (volume equal to 40 times the weight of the

amide in g.) boiled until solution occurred, the warm solution treated with

POCl<sub>3</sub> (volume in cc. equal to twice the weight of the amide: the solution

refluxed

2-3 h. after the spontaneous reaction subsided, cooled, diluted with 15

vols. pentane, and filtered, the precipitate dissolved in the min. amount hot

absolute



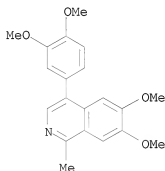
EtOH, the hot solution treated with solid KOH until a strong alkaline reaction persisted, cooled, and diluted with cold H<sub>2</sub>O until no further separation occurred, the product extracted with Et<sub>2</sub>O-EtOAc (2-4 portions), and the extract washed with 2 portions H<sub>2</sub>O, dried, and evaporated at 70° gave the desired 3,4-dihydroisoquinoline (XXIV). The XXIV, an equal weight 10% Pd-C, and p-cymene (volume in cc. equal to 100 times the weight of the XXIV)

distilled

until the reflux temperature reached 175°, the residual mixture refluxed 2-4 h. and filtered hot, the filtrate recharged with the catalyst, refluxed 3 h., filtered, and evaporated, and the resulting isoquinoline recrystd.; if the product did not crystallize, it was dissolved in MeOHEtOAc and treated with dry HCl to give the crystalline HCl salt. XVIII (7.0 g.) cyclized in this manner, and the resulting brown, viscous oily XXIV (3.0 g.) dehydrogenated and triturated with MeOH gave 1.2 g. (18%) 3-(3,4-dimethoxyphenyl)-6,7-dimethoxyisoquinoline (II), m. 204-9° (recrystd. from MeOH, brilliant, pale-yellow leaflets, m. 212-14°),  $\lambda_{\text{maximum}}$  6.15  $\mu$ ; HCl salt, yellow crystals, m. 232-5° (from MeOH),  $\lambda_{\text{maximum}}$  6.15  $\mu$ , showed at 50 mg./kg. a slow fall of the blood pressure, at 15 mg./kg., partial TMA block; the fatal dose was above 50 mg./kg. II refluxed 3 h. with EtI did not give an ethiodide. XXI (4.5 g.) cyclized and the product triturated with MeOH yielded 3.5 g. (82%) 3,4-dihydro derivative (XXV) of III, discolored crystals, m. 75-80° (recrystd. from MeOH, colorless crystals, m. 87-9°),  $\lambda_{\text{CHCl}_3\text{max}}$  6.14  $\mu$ , soluble in dilute HCl. XXV (3.5 g.) dehydrogenated in the usual manner, and the product triturated with MeOH yielded 1.4 g. (40%) III, crystals, m. 205-7° (recrystd. from MeOH, pale greenish yellow crystals, m. 206-8°),  $\lambda_{\text{CHCl}_3\text{max}}$  6.14  $\mu$ ; HCl salt hemihydrate, pale yellow needles, m. 206-7° (decomposition) (dried in vacuo at 80°), 3.0 mg./kg. and up caused a sustained fall of the blood pressure, 31 mg./kg. gave epinephrine block and TMA block and caused convulsions and tachycardia; the fatal dose was above 63 mg./kg. III refluxed 1.5 h. with a large excess EtI, and the gradually separating yellow crystals recrystd. from MeOH gave III.MeI, bright yellow crystals, m. 219-23° (decomposition), which could not be analyzed successfully because of its hygroscopic properties; 7.0 mg./kg. cause a slight and 15 mg./kg. a marked fall of blood pressure; 7 mg./kg. gave an epinephrine shock with rapid recovery and a partial TMA block, and also caused tachycardia; the fatal dose was 76 mg./kg. XXII (19.5 g.) cyclized gave 18 g. viscous, red oil ( $\lambda_{\text{maximum}}$  5.80, 6.15  $\mu$ ; soluble in dilute HCl); a 17-g. portion dehydrogenated in the usual manner, the resulting greenish glassy substance remaining after the evaporation of the p-cymene dissolved in MeOH-EtOAc, the solution treated with cooling with dry HCl, and the crystalline precipitate recrystd. from EtOAc containing the min. amount MeOH yielded 6.5 g. (33%) IV.HCl.0.5H<sub>2</sub>O, m. 173-5° (recrystd. from EtOAc-MeOH, colorless needles, m. 183-5° (decomposition) (dried in vacuo at 80°); 7.0 mg. caused a moderate, transient fall of blood pressure, 31 mg./kg. gave a TMA and a partial epinephrine block, fatal dose above 57 mg. 3,4-(MeO)2C6H3(CH2)2NHAc (14.2 g.) cyclized gave 3.6 g. (26%) 1-methyl-6,7-dimethoxy-3,4-dihydroisoquinoline (XXVI), m. 85-96° (recrystd. from cyclohexane, m. 102-4°),  $\lambda_{\text{maximum}}$  6.15  $\mu$ , moderately soluble in H<sub>2</sub>O. XXVI (3.2 g.) dehydrogenated gave a green glassy material which treated with HCl in MeOH-EtOAc and cooled yielded 2.5 g. (67%) V.HCl, m. 219-221° (decomposition) [recrystd. from MeOH-EtOAc, colorless crystals having a green cast, m. 226-8° (decomposition)]; 3.0 mg./kg. showed a slight and 31 mg. a moderate, sustained fall of blood

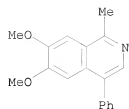
pressure, 53 mg./kg. gave an epinephrine and a TMA block; the fatal dose was above 53 mg./kg. XXVI (7.2 g.) cyclized gave 6.2 g. (91%) discolored crystals, m. 157-60°, which recrystd. from EtOAc gave the 7,8,15,16-tetrahydro derivative (XXVII) of VI, colorless crystals with a green-yellow cast, m. 160-2°,  $\lambda_{CHCl_3}$  max. 6.21, 6.07, 6.18  $\mu$ . Crude XXVII (2.3 g.) dehydrogenated and the product triturated with MeOH yielded 1.6 g. (70%) VI, crystals, m. 191-3°,  $\lambda_{CHCl_3}$  max. 6.18  $\mu$ ; HCl salt, yellow needles, m. 224-5° (from MeOH), readily soluble in H<sub>2</sub>O; 1.0 mg./kg. and up gave a moderate fall of blood pressure, 7.0 mg./kg. and up caused a partial epinephrine block, 15 mg./kg. a partial TMA block; the fatal dose was above 31 mg./kg. VI refluxed 3 h. with EtI gave the VI.MeI which warmed with MeOH gave VI. XXVII in glacial AcOH hydrogenated 1 h. at 40 lb. pressure and 70° over 5% Pd-C, and the resulting semicryst., hygroscopic material triturated with EtOAc, treated in MeOH-EtOAc with dry HCl, and recrystd. from MeOH gave 5,6,7,8,15,16-hexahydro derivative of VI, colorless crystals, m. 263-5°. XX (22 g.) refluxed 4 h. in 500 cc. dry PhMe with 40 cc. POCl<sub>3</sub>, the product isolated in the usual manner, and the resulting partially crystallized material (11 g.) triturated and recrystd. with MeOH gave 4.5 g. colorless crystals, m. 157-9°; the filtrate evaporated gave a glassy residue; both products were free of N but seemed to contain a small amount nonnitrogenous impurity;  $\lambda_{\text{maximum}}$  6.22-6.27  $\mu$  (doublet); the product was presumably (3,4-C<sub>6</sub>H<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>.

IT 102012-79-3, Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (and derivs.)  
 RN 102012-79-3 HCAPLUS  
 CN Isoquinoline, 4-(3,4-dimethoxyphenyl)-6,7-dimethoxy-1-methyl- (CA INDEX NAME)



IT 6286-58-4P, Isoquinoline, 6,7-dimethoxy-1-methyl-4-phenyl-, hydrochloride 790595-06-1P, Isoquinoline, 6,7-dimethoxy-1-methyl-4-phenyl- 855717-78-1P, Isoquinolinium, 4-(3,4-dimethoxyphenyl)-2-ethyl-6,7-dimethoxy-1-methyl-, iodide  
 RL: PREP (Preparation)  
 (preparation of)  
 RN 6286-58-4 HCAPLUS  
 CN Isoquinoline, 6,7-dimethoxy-1-methyl-4-phenyl-, hydrochloride (9CI) (CA INDEX NAME)

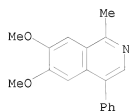
stn



● HCl

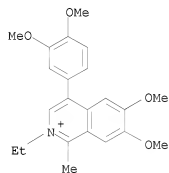
RN 790595-06-1 HCAPLUS

CN Isoquinoline, 6,7-dimethoxy-1-methyl-4-phenyl- (CA INDEX NAME)



RN 855717-78-1 HCAPLUS

CN Isoquinolinium, 4-(3,4-dimethoxyphenyl)-2-ethyl-6,7-dimethoxy-1-methyl-, iodide (1:1) (CA INDEX NAME)



● I<sup>-</sup>

=> file caold  
COST IN U.S. DOLLARS

SINCE FILE TOTAL  
ENTRY SESSION

Updated Search

stn

FULL ESTIMATED COST	174.19	354.14
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
CA SUBSCRIBER PRICE	ENTRY	SESSION
	-23.20	-23.20

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FILE COVERS 1907-1966  
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

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=> d his

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FILE 'REGISTRY' ENTERED AT 06:01:29 ON 08 DEC 2008

L1 STRUCTURE UPLOADED  
L2 15 S L1  
L3 277 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 06:04:08 ON 08 DEC 2008

L4 29 S L3  
L5 4 S L4 AND TROTTER, B?/AU  
L6 25 S L4 NOT L5  
L7 0 S L6 AND NANDA, K?/AU  
L8 0 S L6 AND KETT, N?/AU  
L9 0 S L6 AND DINSMORE, C?/AU  
L10 0 S L6 AND PONTICELLO, G?/AU  
L11 0 S L6 AND CLAREMON, D?/AU

Updated Search

stn

FILE 'CAOLD' ENTERED AT 06:07:28 ON 08 DEC 2008

=> s l3

L12 3 L3

=> d l12, all, 1-3

L12 ANSWER 1 OF 3 CAOLD COPYRIGHT 2008 ACS on STN

AN CA52:9128d CAOLD

TI synthesis of derivs. of 4-(3',4'-dimethoxyphenyl)-6,7-dimethoxyisoquinoline

AU Quelet, Raymond; Mansouri, M.; Pineau, R.

IT 23230-74-2 87519-61-7 102010-96-8 102012-78-2  
102012-79-3 102373-21-7 102597-96-6 102891-93-0  
102948-36-7 103271-78-9 103271-79-0 109980-28-1 110149-36-5  
111719-66-5 114399-21-2 114553-25-2 114791-79-6  
114839-77-9 115387-73-0 115485-51-3

L12 ANSWER 2 OF 3 CAOLD COPYRIGHT 2008 ACS on STN

AN CA52:7320a CAOLD

TI cyclic nitrones - (II) polymers of 2,3,4,5-tetrahydropyridine-N-oxide and related compds.

AU Thesing, Jan; Mayer, H.

IT 3146-87-0 24423-87-8 34418-91-2 54105-63-4 54105-64-5  
67787-56-8 86601-68-5 94269-66-6 98995-80-3 100881-81-0  
101093-12-3 101273-53-4 101442-06-2 101583-92-0 102468-41-7  
102593-23-7 102593-24-8 102593-25-9 102598-82-3 102890-40-4  
102890-41-5 102890-42-6 102890-43-7 108757-10-4 108973-36-0  
112685-68-4 116535-45-6

L12 ANSWER 3 OF 3 CAOLD COPYRIGHT 2008 ACS on STN

AN CA52:7319h CAOLD

TI syntheses of isoquinoline derivs. of pharmacol. interest

AU Deshpande, V. N.; Nargund, K. S.

IT 22251-34-9 102010-96-8 102890-46-0 102890-47-1 102952-43-2  
109614-11-1 113751-11-4

=> file reg

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	11.73	365.87
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	0.00	-23.20

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DICTIONARY FILE UPDATES: 5 DEC 2008 HIGHEST RN 1080697-25-1

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E4	1	82894-70-0/RN
E5	1	82894-71-1/RN
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E7	1	82894-73-3/RN
E8	1	82894-74-4/RN
E9	1	82894-75-5/RN
E10	1	82894-76-6/RN
E11	1	82894-77-7/RN
E12	1	82894-78-8/RN

=> s e3

L13 1 82894-69-7/RN

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
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FULL ESTIMATED COST	0.46	366.33
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L14      0 L13/USES
          (L13 (L) USES/RL)
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FULL ESTIMATED COST                5.38        371.71

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CA SUBSCRIBER PRICE                0.00        -23.20
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DICTIONARY FILE UPDATES: 5 DEC 2008 HIGHEST RN 1080697-25-1

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stn

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E8	1	374594-14-6/RN
E9	1	374594-15-7/RN
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E11	1	374594-17-9/RN
E12	1	374594-18-0/RN

=> s e3

L15 1 374594-09-9/RN

=> file hcaplus

COST IN U.S. DOLLARS

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FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
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=> s l15/uses

1 L15
7317060 USES/RL
L16 0 L15/USES
(L15 (L) USES/RL)

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FULL ESTIMATED COST	2.69	374.86
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
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=>  
Uploading C:\Documents and Settings\brobinson1\My Documents\adfnatit.str

L17 STRUCTURE UPLOADED

=> s l17  
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SAMPLE SCREEN SEARCH COMPLETED - 79 TO ITERATE

100.0% PROCESSED 79 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 1047 TO 2113  
PROJECTED ANSWERS: 1 TO 80

L18 1 SEA SSS SAM L17

=> s l17 full  
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

Updated Search

stn

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
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FULL SCREEN SEARCH COMPLETED - 1429 TO ITERATE

100.0% PROCESSED 1429 ITERATIONS 10 ANSWERS  
SEARCH TIME: 00.00.01

L19 10 SEA SSS FUL L17

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	ENTRY	SESSION
FULL ESTIMATED COST	178.82	553.68
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	0.00	-23.20

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7317060 USES/RL  
L20 2 L19/USES  
(L19 (L) USES/RL)

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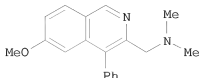
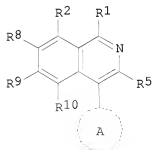
L20 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2005:300191 HCAPLUS  
DOCUMENT NUMBER: 142:373697

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stn

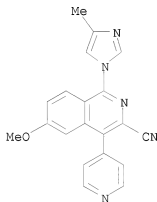
TITLE: Preparation of isoquinoline derivatives as potassium channel inhibitors  
 INVENTOR(S): Trotter, B. Wesley; Nanda, Kausik K.; Kett, Nathan R.; Dinsmore, Christopher J.; Ponticello, Gerald S.; Claremon, David A.  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
 SOURCE: PCT Int. Appl., 115 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005030130	A2	20050407	WO 2004-US30486	20040917
WO 2005030130	A3	20060119		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004275720	A1	20050407	AU 2004-275720	20040917
AU 2004275720	B2	20080424		
CA 2539479	A1	20050407	CA 2004-2539479	20040917
EP 1667979	A2	20060614	EP 2004-784370	20040917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR CN 1856475 A 20061101 CN 2004-80027385 20040917 JP 2007506743 T 20070322 JP 2006-528072 20040917 IN 2006DN00877 A 20070810 IN 2006-DN877 20060220 US 20060276450 A1 20061207 US 2006-572342 20060317 US 2003-505143P US 2003-505143P P 20030923 WO 2004-US30486 W 20040917				
PRIORITY APPLN. INFO.: OTHER SOURCE(S): CASREACT 142:373697; MARPAT 142:373697 GI				



stn

- AB Title compds. represented by the formula I [wherein ring A = (un)substituted (hetero)aryl or heterocyclic ring; R1 = H, CN, halo, (alkyl)amino, etc.; R2, R8-R10 = independently H, halo, aminocarbonyl, etc.; R5 = H, halo, (cyclo)alkyl, etc.; and pharmaceutically acceptable salts, crystal forms or hydrates thereof] were prepared as potassium channel inhibitors. For example, Ni-catalyzed reduction of 1-chloro-6-methoxy-4-phenylisoquinoline-3-carbonitrile and followed by condensation with formaldehyde, gave II•2HCl. I provided  $\geq 50\%$  inhibition at concentration  $\leq 33 \mu\text{M}$  in the high-throughput Kv1.5 planar patch clamp assay and  $\geq 25\%$  inhibition at concentration  $\leq 25 \mu\text{M}$  in the AAS (atomic absorption spectroscopy) assay. Thus, I and their pharmaceutical compns. are useful as potassium channel inhibitors for the treatment of cardiac arrhythmias, and the like.
- IT 849548-32-9P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of isoquinoline derivs. as potassium channel inhibitors)
- RN 849548-32-9 HCAPLUS
- CN 3-Isoquinolinecarbonitrile, 6-methoxy-1-(4-methyl-1H-imidazol-1-yl)-4-(4-pyridinyl)- (CA INDEX NAME)



L20 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:398243 HCAPLUS

DOCUMENT NUMBER: 129:81741

ORIGINAL REFERENCE NO.: 129:16880h,16881a

TITLE: Preparation of pyridines as antiasthmatics

INVENTOR(S): Ukita, Tatsuzo; Sugahara, Masakatsu; Ikezawa, Katsuo; Kikkawa, Hideo; Naito, Kazuaki

PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 59 pp.  
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 848000	A1	19980617	EP 1997-309947	19971210
EP 848000	B1	20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 5965730	A	19991012	US 1997-985042	19971204
TW 429257	B	20010411	TW 1997-86118300	19971205
AT 219075	T	20020615	AT 1997-309947	19971210
PT 848000	T	20020930	PT 1997-309947	19971210
ES 2178741	T3	20030101	ES 1997-309947	19971210
CA 2224635	A1	19980613	CA 1997-2224635	19971211
CA 2224635	C	20060131		
CN 1184813	A	19980617	CN 1997-125491	19971212
CN 1127498	C	20031112		
JP 10226685	A	19980825	JP 1997-342352	19971212
JP 3951395	B2	20070801		
HK 1012505	A1	20021025	HK 1998-113891	19981217
PRIORITY APPLN. INFO.:			JP 1996-333357	A 19961213
OTHER SOURCE(S):	MARPAT 129:81741			
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

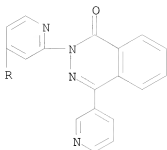
AB The title compds. [I; A = II-VI (wherein R1, R2 = H, (un)protected OH; R31, R41, R42 = (un)protected CH2OH; R32 = H, lower alkyl, (un)protected CH2OH; R33 = (un)substituted lower alkyl; the dotted line means the presence or absence of a double bond); R5, R6 = H, (un)protected NH2, or NR5R6 = (un)substituted heterocycle], which show excellent bronchoconstriction inhibitory activity and/or anti-inflammatory activity of airways, and therefore are useful in the prophylaxis or treatment of asthma, were prepared. Thus, reaction of 4-(3-pyridyl)phthalazin-1(2H)-one with 2-bromo-4-[6,7-dimethoxy-2-(4-pyridyl)methyl]phthalazin-1(2H)-on-4-yl]pyridine in the presence of K2CO3 and CuI in DMF afforded the title compound VII. Compds. I are effective at 0.003-3 mg/kg/day.

IT 209261-51-8P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyridines as antiasthmatics)

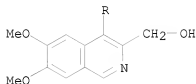
RN 209261-51-8 HCAPLUS

CN 1(2H)-Phthalazinone, 2-[4-[3-(hydroxymethyl)-6,7-dimethoxy-4-isoquinolinyl]-2-pyridinyl]-4-(3-pyridinyl)-, hydrochloride (1:1) (CA INDEX NAME)

stn



● HCl



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

=> file caold

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
94.29	647.97

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
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-1.60	-24.80

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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- . November 22, 2008 - removed from database clusters
- . December 31, 2008 - removed from STN

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FILE 'REGISTRY' ENTERED AT 06:01:29 ON 08 DEC 2008

L1 STRUCTURE UPLOADED  
L2 15 S L1  
L3 277 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 06:04:08 ON 08 DEC 2008

L4 29 S L3  
L5 4 S L4 AND TROTTER, B?/AU  
L6 25 S L4 NOT L5  
L7 0 S L6 AND NANDA, K?/AU  
L8 0 S L6 AND KETT, N?/AU  
L9 0 S L6 AND DINSMORE, C?/AU  
L10 0 S L6 AND PONTICELLO, G?/AU  
L11 0 S L6 AND CLAREMON, D?/AU

FILE 'CAOLD' ENTERED AT 06:07:28 ON 08 DEC 2008

L12 3 S L3

FILE 'REGISTRY' ENTERED AT 06:19:47 ON 08 DEC 2008

E 82894-69-7/RN  
L13 1 S E3

FILE 'HCAPLUS' ENTERED AT 06:19:59 ON 08 DEC 2008

L14 0 S L13/USES

FILE 'REGISTRY' ENTERED AT 06:21:25 ON 08 DEC 2008

E 374594-09-9/RN  
L15 1 S E3

FILE 'HCAPLUS' ENTERED AT 06:21:45 ON 08 DEC 2008

L16 0 S L15/USES

FILE 'REGISTRY' ENTERED AT 06:22:28 ON 08 DEC 2008

L17 STRUCTURE UPLOADED  
L18 1 S L17  
L19 10 S L17 FULL

FILE 'HCAPLUS' ENTERED AT 06:23:30 ON 08 DEC 2008

L20 2 S L19/USES

FILE 'CAOLD' ENTERED AT 06:42:18 ON 08 DEC 2008

Updated Search

stn

=> s l19

L21 0 L19

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.46

648.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

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0.00

-24.80

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DICTIONARY FILE UPDATES: 5 DEC 2008 HIGHEST RN 1080697-25-1

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

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L22 STRUCTURE UPLOADED

=> s l22

SAMPLE SEARCH INITIATED 06:46:01 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 131 TO ITERATE

100.0% PROCESSED 131 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1934 TO 3306

PROJECTED ANSWERS: 1 TO 80

L23

1 SEA SSS SAM L22

Updated Search



stn

=> s l22 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS

DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y

FULL SEARCH INITIATED 06:46:05 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 2371 TO ITERATE

100.0% PROCESSED 2371 ITERATIONS

10 ANSWERS

SEARCH TIME: 00.00.01

L24

10 SEA SSS FUL L22